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A (FORGOTTEN) UPPER BOUND FOR THE SPECTRAL RADIUS OF A GRAPH

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Abstract. The best degree-based upper bound for the spectral radius is due to Liu and Weng. This paper begins by demonstrating that a (forgotten) upper bound for the spectral radius dating from 1983 is equivalent to their much more recent bound. This bound is then used to compare lower bounds for the clique number. A series of line graph degree-based upper bounds for the Q-index is then proposed and compared experimentally with a graph based bound. Finally a new lower bound for generalised r-partite graphs is proved, by extending a result due to Erdös.

1. Introduction

Let G be a simple and undirected graph with n vertices, m edges, and degrees $\Delta = d_1 \geq d_2 \geq \cdots \geq d_n = \delta$. Let d denote the average vertex degree, ω the clique number and χ the chromatic number. Finally let $\mu(G)$ denote the spectral radius of G, $q(G)$ denote the spectral radius of the signless Laplacian of G and G^L denote the line graph of G.

In 1983, Edwards and Elphick [6] proved in their Theorem 8 (and its corollary) that $\mu \leq y - 1$, where y is defined by the equality

$$y(y-1) = \sum_{k=1}^{\lfloor y \rfloor} d_k + (y - \lfloor y \rfloor) d_{\lceil y \rceil}. \tag{1}$$

Edwards and Elphick [6] show that $1 \leq y \leq n$ and that y is a single-valued function of G.

This bound is exact for regular graphs because, we then have that

$$d = \mu \leq y - 1 = \frac{1}{y}\left(\sum_{k=1}^{\lfloor y \rfloor} d + (y - \lfloor y \rfloor) d\right) = d.$$

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The bound is also exact for various bidegreed graphs. For example, let G be the Star graph on n vertices, which has $\mu = \sqrt{n-1}$. It is easy to show that $\lfloor \sqrt{n-1} \rfloor < y < \lceil \sqrt{n-1} \rceil$. It then follows that y is the solution to the equation

$$y(y-1) = (n-1) + \lfloor \sqrt{n-1} \rfloor - 1 + (y - \lfloor \sqrt{n-1} \rfloor) = n - 2 + y,$$

which has the solution $y = 1 + \sqrt{n-1}$, so $\mu \le y - 1 = \sqrt{n-1}$.

Similarly let G be the Wheel graph on n vertices, which has $\mu = 1 + \sqrt{n}$. It is straightforward to show that $y = 2 + \sqrt{n}$ is the solution to (1) so again the bound is exact.

2. An Upper Bound for the Spectral Radius

The calculation of y can involve a two step process.

1. Restrict y to integers, so (1) simplifies to

$$y(y-1) = \sum_{k=1}^{y} d_k.$$

Since $d \le \mu$, we can begin with $y = \lfloor d + 1 \rfloor$, and then increase y by unity until $y(y-1) \ge \sum_{k=1}^{y} d_k$. This determines that either $y = a$ or $a < y < a+1$, where a is an integer.

2. Then, if y is not an integer, solve the following quadratic equation

$$y(y-1) = \sum_{k=1}^{a} d_k + (y-a) d_{a+1}. \tag{2}$$

For convenience let $c = \sum_{k=1}^{a} d_k$. Equation (2) then becomes

$$y^2 - y(1 + d_{a+1}) - (c - a d_{a+1}) = 0.$$

Therefore

$$y = \frac{d_{a+1} + 1 + \sqrt{(d_{a+1}+1)^2 + 4(c - a d_{a+1})}}{2}$$

so

$$\mu \le y - 1 = \frac{d_{a+1} - 1 + \sqrt{(d_{a+1}+1)^2 + 4(c - a d_{a+1})}}{2}.$$

This two step process can be combined as follows, by letting $a + 1 = k$,

$$\mu \le \frac{d_k - 1 + \sqrt{(d_k+1)^2 + 4\sum_{i=1}^{k-1}(d_i - d_k)}}{2}, \text{ where } 1 \le k \le n. \tag{3}$$

In 2012, Liu and Weng [12] proved (3) using a different approach. They also proved there is equality if and only if G is regular or there exists $2 \leq t \leq k$ such that $d_1 = d_{t-1} = n - 1$ and $d_t = d_n$. Note that if $k = 1$ this reduces to $\mu \leq \Delta$.

If we set $k = n$ in (3) then

$$\mu \leq \frac{\delta - 1 + \sqrt{(\delta + 1)^2 - 4n\delta + 8m}}{2}$$

which was proved by Nikiforov [13] in 2002.

3. Lower Bounds for the Clique Number

Turán's Theorem, proved in 1941, is a seminal result in extremal graph theory. In its concise form it states that:

$$\frac{n}{n-d} \leq \omega(G)$$

where d is the average vertex degree.

Edwards and Elphick [6] used y to prove the following lower bound for the clique number:

$$\frac{n}{n-y+1} < \omega(G) + \frac{1}{3}. \tag{4}$$

In 1986, Wilf [16] proved that

$$\frac{n}{n-\mu} \leq \omega(G).$$

Note, however, that

$$\frac{n}{n-y+1} \not\leq \omega(G),$$

since for example $\frac{n}{n-y+1} = 2.13$ for $K_{7,9}$ and $\frac{n}{n-y+1} = 3.1$ for $K_{3,3,4}$.

Nikiforov [13] proved a conjecture due to Edwards and Elphick [6] that

$$\frac{2m}{2m-\mu^2} \leq \omega(G). \tag{5}$$

Experimentally, bound (5) performs better than bound (4) for most graphs.

4. Upper Bounds for the Q-Index

Let $q(G)$ denote the spectral radius of the signless Laplacian of G. In this section we investigate graph and line graph degree-based bounds for $q(G)$ and then compare them experimentally.

4.1. Graph bound

Nikiforov [14] has recently strengthened various upper bounds for $q(G)$ with the following theorem.

Theorem 1. *If G is a graph with n vertices, m edges, with maximum degree Δ and minimum degree δ, then*

$$q(G) \leq \min\left(2\Delta, \frac{1}{2}\left(\Delta + 2\delta - 1 + \sqrt{(\Delta + 2\delta - 1)^2 + 16m - 8(n - 1 + \Delta)\delta}\right)\right).$$

Equality holds if and only if G is regular or G has a component of order $\Delta + 1$ in which every vertex is of degree δ or Δ, and all other components are δ-regular.

4.2. Line graph bounds

The following well-known lemma (see, for example, Lemma 2.1 in [2]) provides an equality between the spectral radii of the signless Laplacian matrix and the adjacency matrix of the line graph of a graph.

Lemma 2. *If G^L denotes the line graph of G then*

$$q(G) = 2 + \mu(G^L). \tag{6}$$

Let $\Delta_{ij} = \{d_i + d_j - 2 \mid i \sim j\}$ be the degrees of vertices in G^L, and $\Delta_1 \geq \Delta_2 \geq \cdots \geq \Delta_m$ be a renumbering of them in non-increasing order. Cvetković *et al.* proved the following theorem using Lemma 2.

Theorem 3. (Theorem 4.7 in [4]).

$$q(G) \leq 2 + \Delta_1$$

with equality if and only if G is regular or semi-regular bipartite.

The following lemma is proved in varying ways in [5, 12, 15].

Lemma 4.

$$\mu(G) \leq \frac{d_2 - 1 + \sqrt{(d_2 - 1)^2 + 4d_1}}{2}$$

with equality if and only if G is regular or $n - 1 = d_1 > d_2 = d_n$.

Chen *et al.* combined Lemma 2 and Lemma 4 to prove the following result.

Theorem 5. (Theorem 3.4 in [3]).

$$q(G) \leq 2 + \frac{\Delta_2 - 1 + \sqrt{(\Delta_2 - 1)^2 + 4\Delta_1}}{2}$$

with equality if and only if G is regular, or semi-regular bipartite, or the tree obtained by joining an edge to the centers of two stars $K_{1,\frac{n}{2}-1}$ with even n, or $n - 1 = d_1 = d_2 > d_3 = d_n = 2$.

Stating (3) as a lemma we have

Lemma 6. *For* $1 \le k \le n$,

$$\mu(G) \le \phi_k := \frac{d_k - 1 + \sqrt{(d_k+1)^2 + 4\sum_{i=1}^{k-1}(d_i - d_k)}}{2} \tag{7}$$

with equality if and only if G *is regular or there exists* $2 \le t \le k$ *such that* $n-1 = d_1 = d_{t-1} > d_t = d_n$.

Combining Lemmas 2 and 6 provides the following series of upper bounds for the signless Laplacian spectral radius.

Theorem 7. *For* $1 \le k \le m$, *we have*

$$q(G) \le \psi_k := 1 + \frac{\Delta_k + 1 + \sqrt{(\Delta_k+1)^2 + 4\sum_{i=1}^{k-1}(\Delta_i - \Delta_k)}}{2} \tag{8}$$

with equality if and only if $\Delta_1 = \Delta_m$ *or there exists* $2 \le t \le k$ *such that* $m-1 = \Delta_1 = \Delta_{t-1} > \Delta_t = \Delta_m$.

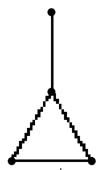
Proof. G^L is simple. Hence (8) is a direct result of (6) and (7). The sufficient and necessary conditions are immediately those in Lemma 6. ■

Remark 8. Note that Theorem 7 generalizes both Theorems 3 and 5 since those bounds are precisely ψ_1 and ψ_2 in (8) respectively.

We list all the extremal graphs with equalities in (8) in the following. From Theorem 3 the graphs with $q(G) = \psi_1$, i.e. $\Delta_1 = \Delta_m$, are regular or semi-regular bipartite.

From Theorem 5 the graphs with $q(G) < \psi_1$ and $q(G) = \psi_2$, i.e. $m-1 = \Delta_1 > \Delta_2 = \Delta_m$, are the tree obtained by joining an edge to the centers of two stars $K_{1,\frac{n}{2}-1}$ with even n, or $n-1 = d_1 = d_2 > d_3 = d_n = 2$.

The only graph with $q(G) < \min\{\psi_i \mid i = 1,2\}$ and $q(G) = \psi_3$, i.e. $m-1 = \Delta_1 = \Delta_2 > \Delta_3 = \Delta_m$, is the 4-vertex graph $K_{1,3}^+$ obtained by adding one edge to $K_{1,3}$.



$K_{1,3}^+$

We now prove that no graph satisfies $q(G) < \min\{\psi_i \mid 1 \le i < k-1\}$ and $q(G) = \psi_k$ where $m \ge k \ge 4$. Let G be a counter-example such that $m-1 = \Delta_1 = \Delta_{k-1} > \Delta_k = \Delta_m$. Since $\Delta_3 = m-1$ there are at least 3 edges incident to all other edges in G. If these 3 edges form a 3-cycle then there is nowhere to place the fourth edge, which is a contradiction. Hence they are incident to a common vertex, and G has to be a star graph. However a star graph is semi-regular bipartite so $q(G) = \psi_1$, which completes the proof.

Remark 9. By analogy with (1), if z is defined by the equality

$$z(z-1) = \sum_{k=1}^{\lfloor z \rfloor} \Delta_k + (z - \lfloor z \rfloor)\Delta_{\lceil z \rceil},$$

then $q \leq z + 1$. This bound is exact for $d-$regular graphs, because we then have

$$2d = q \leq z + 1 = 2 + (z-1) = 2 + \frac{1}{z}\left(\sum_{k=1}^{\lfloor z \rfloor} \Delta + (z - \lfloor z \rfloor)\Delta\right) = 2 + \Delta = 2d.$$

4.3. Experimental comparison

It is straightforward to compare the above bounds experimentally using the named graphs and LineGraph function in Wolfram Mathematica. Theorem 1 is exact for some graphs (eg Wheels) for which Theorems 5 and 7 are inexact and Theorems 5 and 7 are exact for some graphs (eg complete bipartite) for which Theorem 1 is inexact. Tabulated below are the numbers of named irregular graphs on 10, 16, 25 and 28 vertices in `Mathematica` and the average values of q and the bounds in Theorems 1, 5 and 7.

n	irrregular graphs	$q(G)$	Theorem 1	Theorem 5	Theorem 7
10	59	9.3	10.0	10.3	9.8
16	48	10.3	11.2	11.5	11.0
25	25	11.5	13.4	13.1	12.6
28	21	11.2	12.6	12.7	12.2

It can be seen that Theorem 5 gives results that are broadly equal on average to Theorem 1 and Theorem 7 gives results which are on average modestly better. This is unsurprising since more data is involved in Theorem 7 than in the other two theorems. For some graphs, $q(G)$ is minimised in Theorem 7 with large values of k.

5. A Lower Bound for the Q-Index

Elphick and Wocjan [7] defined a measure of graph irregularity, ν, as follows:

$$\nu = \frac{n \sum d_i^2}{4m^2},$$

where $\nu \geq 1$, with equality only for regular graphs.

It is well known that $q \geq 2\mu$ and Hofmeister [9] has proved that $\mu^2 \geq \sum d_i^2/n$, so it is immediate that

$$q \geq 2\mu \geq \frac{4m\sqrt{\nu}}{n}.$$

Liu and Liu [11] improved this bound in the following theorem, for which we provide a simpler proof using Lemma 2.

Theorem 10. *Let G be a graph with irregularity ν and Q-index $q(G)$. Then*

$$q(G) \geq \frac{4m\nu}{n}.$$

This is exact for complete bipartite graphs.

Proof. Let G^L denote the line graph of G. From Lemma 2 we know that $q(G) = 2 + \mu(G^L)$ and it is well known that $n(G^L) = m$ and $m(G^L) = (\sum d_i^2/2) - m$. Therefore

$$q = 2 + \mu(G^L) \geq 2 + \frac{2m(G^L)}{n(G^L)} = 2 + \frac{2}{m}\left(\frac{\sum d_i^2}{2} - m\right) = \frac{\sum d_i^2}{m} = \frac{4m\nu}{n}.$$

For the complete bipartite graph $K_{s,t}$,

$$q \geq \frac{\sum_i d_i^2}{m} = \frac{\sum_{ij \in E}(d_i + d_j)}{m} = d_i + d_j = s + t = n,$$

which is exact. ■

6. Generalised r-Partite Graphs

In a series of papers, Bojilov and others have generalised the concept of an r-partite graph. They define the parameter $\phi(G)$ to be the smallest integer r for which $V(G)$ has an r-partition:

$$V(G) = V_1 \cup V_2 \cup \cdots \cup V_r, \text{ such that } d(v) \leq n - n_i, \text{ where } n_i = |V_i|,$$

for all $v \in V_i$ and for $i = 1, 2, \ldots, r$.

Bojilov *et al.* [1] proved that $\phi(G) \leq \omega(G)$ and Khadzhiivanov and Nenov [10] proved that

$$\frac{n}{n-d} \leq \phi(G).$$

Despite this bound, Elphick and Wocjan [7] demonstrated that

$$\frac{n}{n-\mu} \not\leq \phi(G).$$

However, it is proved below in Corollary 15 that

$$\frac{n}{n-\mu} \leq \frac{n}{n-y+1} < \phi(G) + \frac{1}{3}.$$

Definition 11. If H is any graph of order n with degree sequence $d_H(1) \geq d_H(2) \geq \ldots \geq d_H(n)$, and if H^* is any graph of order n with degree sequence $d_{H^*}(1) \geq d_{H^*}(2) \geq \ldots \geq d_{H^*}(n)$, such that $d_H(i) \leq d_{H^*}(i)$ for all i, then H^* is said to "dominate" H.

Erdös [8] proved that if G is any graph of order n, then there exists a graph G^* of order n, where $\chi(G^*) = \omega(G) = r$, such that G^* dominates G and G^* is complete r-partite.

Theorem 12. *If G is any graph of order n, then there exists a graph G^* of order n, where $\omega(G^*) = \phi(G) = r$, such that G^* dominates G, and G^* is complete r-partite.*

Proof. Let G be a generalised r-partite graph with $\phi(G) = r$ and $n_i = |V_i|$, and let G^* be the complete r-partite graph $K_{n_1,\ldots,n_r}$. Let $d(v)$ denote the degree of vertex v in G and $d^*(v)$ denote the degree of vertex v in G^*. Clearly $\chi(G^*) = \omega(G^*) = r$, and by the definition of a generalised r-partite graph:

$$d^*(v) = n - n_i \geq d(v)$$

for all $v \in V_i$ and for $i = 1, \ldots, r$. Therefore G^* dominates G. ∎

Lemma 13. (Lemma 4 in [6]). Assume G^* dominates G. Then $y(G^*) \geq y(G)$.

Theorem 14.

$$\frac{n}{n-y(G)+1} < \phi(G) + \frac{1}{3}.$$

Proof. Let G^* be any graph of order n, where $\omega(G^*) = \phi(G)$ such that G^* dominates G. (By Theorem 12 at least one such graph G^* exists.) Then, using Lemma 13 and inequality (4),

$$\frac{n}{n-y(G)+1} \leq \frac{n}{n-y(G^*)+1} < \omega(G^*)+\frac{1}{3} = \phi(G)+\frac{1}{3} \leq \omega(G)+\frac{1}{3}.$$ ∎

Corollary 15.

$$\frac{n}{n-\mu} < \phi(G) + \frac{1}{3}.$$

Proof. Immediate since $\mu \leq y - 1$. ∎

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