A (forgotten) upper bound for the spectral radius of a graph

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October 7, 2014

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 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 Erdős.

1 Introduction

Let $G$ be a simple and undirected graph with $n$ vertices, $m$ edges, and degrees $\Delta = d_1 \geq d_2 \geq ... \geq d_n = \delta$. Let $d$ denote the average vertex degree, $\omega$ the clique number and $\chi$ 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:

$$y(y - 1) = \sum_{k=1}^{[y]} d_k + (y - [y])d_{[y]}.$$  

(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:

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

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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 $\mu \leq y - 1 = \sqrt{n-1}$.

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

2. Then, if necessary, solve the following quadratic equation:

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

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

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

Therefore

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

so

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

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

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

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:

\[
\frac{n}{n - d} \leq \omega(G).
\]

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

\[
\frac{n}{n - y + 1} < \omega(G) + \frac{1}{3}.
\] (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:

\[
\frac{2m}{2m - \mu^2} \leq \omega(G).
\] (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 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 \( \Delta \) and minimum degree \( \delta \), 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 \( \delta \) or \( \Delta \), and all other components are \( \delta \)-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:

$$q(G) = 2 + \mu(G^L). \quad (6)$$

Let $\Delta_{ij} = \{d_i + d_j - 2 \mid i \sim j\}$ be the degrees of vertices in $G^L$, and $\Delta_1 \geq \Delta_2 \geq \ldots \geq \Delta_m$ 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 [15, 5, 12].

**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 $1 \leq k \leq n$,

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

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

$$\phi_\ell = \min\{\phi_k \mid 1 \leq k \leq n\}$$

where $3 \leq \ell \leq n$ is the smallest integer such that $\sum_{i=1}^{\ell} d_i < \ell(\ell - 1)$. 


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

**Theorem 7.** For \(1 \leq k \leq m\), we have

\[
q(G) \leq \psi_k := 1 + \frac{\Delta_k + 1 + \sqrt{(\Delta_k + 1)^2 + 4 \sum_{i=1}^{k-1} (\Delta_i - \Delta_k)}}{2}
\]

with equality if and only if \(\Delta_1 = \Delta_m\) or there exists \(2 \leq t \leq k\) such that \(m - 1 = \Delta_1 = \Delta_{t-1} > \Delta_t = \Delta_m\). Furthermore,

\[
\psi_t = \min\{\psi_k \mid 1 \leq k \leq m\}
\]

where \(3 \leq \ell \leq m\) is the smallest integer such that \(\sum_{i=1}^\ell \Delta_i < \ell(\ell - 1)\).

**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 Theorem 3 and Theorem 5 since these bounds are precisely \(\psi_1\) and \(\psi_2\) 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 \(K_{1, \frac{m}{2}-1}\) with even \(n\), or \(n - 1 = d_1 = d_2 > d_3 = d_n = 2\).

The only graph with \(q(G) \leq \min\{\psi_i \mid i = 1, 2\}\) 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 \(K_{1,3}\).

We now prove that no graph satisfies \(q(G) < \min\{\psi_i \mid 1 \leq i \leq k - 1\}\) and \(q(G) = \psi_k\) where \(m \geq k \geq 4\). 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 (11), if \(z\) is defined by the equality

\[
z(z - 1) = \Delta_k + (z - \lfloor z \rfloor)\Delta_k,
\]

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 (e.g., Wheels) for which Theorems 5 and 7 are inexact and Theorems 5 and 7 are exact for some graphs (e.g., 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 | irregular 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, $\nu$, 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 $\nu$ 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.

\[\square\]

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 $\phi$ to be the smallest integer $r$ for which $V(G)$ has an $r$–partition:

$$V(G) = V_1 \cup V_2 \cup \ldots \cup V_r,$$

such that $d(v) \leq n - n_i$, 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:

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

However, it is proved below in Corollary 10 that:

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

Definition

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" $H$.

Erdős 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 11. 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 $G$.  

\[\square\]
Lemma 12. (Lemma 4 in [6])
Assume $G^*$ dominates $G$. Then $y(G^*) \geq y(G)$.

Theorem 13.

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

Proof. Let $G^*$ be any graph of order $n$, where $\omega(G^*) = \phi(G)$ such that $G^*$ dominates $G$. (By Theorem 7 at least one such graph $G^*$ exists.) Then, using Lemma 8:

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

Corollary 14.

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

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

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