CONNECTED GRAPHS OF FIXED ORDER AND SIZE WITH MAXIMAL Q–INDEX: SOME SPECTRAL BOUNDS

Milica Andjelić

Department of Mathematics
University of Aveiro

Signless Laplacian spectra

- Considering a graph G, the matrix $Q(G) = A(G) + D(G)$ is called the **signless Laplacian matrix**, where $A(G)$ is the adjacency matrix of G and $D(G)$ is the diagonal matrix of vertex degrees of G.

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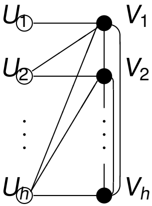
- Considering a graph G, the matrix $Q(G) = A(G) + D(G)$ is called the **signless Laplacian matrix**, where $A(G)$ is the adjacency matrix of G and $D(G)$ is the diagonal matrix of vertex degrees of G.
- The eigenvalues (and the spectrum) of $Q(G)$ are called the **Q-eigenvalues** (resp.) **Q-spectrum** of G, and are written in non-increasing order:

$$\kappa_1(G) \geqslant \kappa_2(G) \geqslant \ldots \geqslant \kappa_n(G).$$

In particular $\kappa_1(G)$ is called the **Q-index** of G.

Nested split graphs I

- Any *nested split graph* G admits a partition of its vertex set into $V_1 \cup \ldots \cup V_h \cup U_1 \cup \ldots \cup U_h$ with following properties:
  - $V_1 \cup \ldots \cup V_h$ induces a clique, and $U_1 \cup \ldots \cup U_h$ induces a co-clique;
  - Each vertex in $u \in U_i$ is adjacent to all vertices $v \in V_1 \cup \ldots \cup V_i$ $(i = 1, \ldots, h)$.



The structure of a connected nested split graph.

Nested split graphs II

The NSG as described can be denoted by $NSG(m_1, m_2, \ldots, m_h; n_1, n_2, \ldots, n_h)$, where $m_i = |U_i|$ and $n_i = |V_i|$ $(i = 1, 2, \ldots, h)$.

Q–eigenvectors of NSGs

For a connected NSG graph G of order n and size m, we set $\kappa = \kappa(G)$ for its Q-index and also we put

- $\kappa_t = \kappa - d_t$, where $d_t = \sum_{i=1}^{t} n_i$ is a vertex degree of any $u \in U_t$,

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- $\bar{\mu}_t$ for $(\kappa - d_t)(\kappa - \bar{d}_1 + 1)$.

It is well known that the Q–eigenvector of G can be taken to be positive. We assume that $\mathbf{x} = (x_1, x_2, \ldots, x_n)^T$ is a Q–eigenvector of G normalized so that $\sum_{i=1}^{n} x_i = 1$. We first observe that all vertices within the sets U_s or V_t $(1 \leq s, t \leq h)$ have the same weights (since they belong to the same orbit of G). Let $x_u = a_s$ if $u \in U_s$, while $x_v = b_t$ if $v \in V_t$.

Q–eigenvectors of NSGs

From the eigenvalue equations for κ (applied on any vertex from U_s, or V_t) we get

$$\kappa a_s = d_s a_s + \sum_{j=1}^{s} n_j b_j \ (s = 1, \ldots, h),$$

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By normalization we have

$$\sum_{i=1}^{h} m_i a_i + \sum_{j=1}^{h} n_j b_j = 1.$$

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$$a_s = \frac{1}{\kappa - d_s} \sum_{j=1}^{s} n_j b_j \ (s = 1, \ldots, h),$$

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We next get

$$(\kappa - d_s)(a_{s+1} - a_s) = n_{s+1}(a_{s+1} + b_{s+1}) \ (s = 0, \ldots, h-1)$$

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$$(\kappa - \bar{d}_1 + 1)(b_1 - b_0) = 1 \; (t = 0),$$

$$(\kappa - \bar{d}_t + 1)(b_{t+1} - b_t) = -m_t(a_t + b_t) \; (t = 1, \ldots, h-1),$$

bearing in mind the following relations $d_{s+1} = d_s + n_s$ and $\bar{d}_t = \bar{d}_{t+1} + m_t$.

q–eigenvectors of NSGs

Since all components of $\mathbf{x}$ are positive and $\kappa \geq \Delta + 1$, where Δ denotes maximum vertex degree in G, we easily get that

$$a_{s+1} > a_s \ (s = 1, \ldots, h-1),$$

$$b_{t+1} < b_t \ (t = 1, \ldots, h-1).$$

In addition, by putting $s = h$ and $t = h$, we get

$$(\kappa - \bar{d}_h + 1)b_h = (\kappa - d_h + m_h)a_h.$$

Since $m_h \geq 1$ and $\bar{d}_h = d_h + m_h - 1$, we also have

$$b_h \geq a_h,$$

where equality holds only in case $m_h = 1$.

We first note that

$$a_1 = \frac{N_1}{\mu_1},\ b_1 = \frac{1}{\bar{\kappa}_1}.$$

Next, we get

$$a_2 = \frac{1}{\mu_2}(N_2 - \frac{n_2 e_1}{\mu_1} + \frac{e_1}{\bar{\kappa}_1}),\ b_2 = \frac{1}{\bar{\kappa}_2}(1 - \frac{e_1}{\mu_1}).$$

Clearly, if we proceed further on in this way then the corresponding expressions become too messy. Therefore, we will next on focus our attention on bounding these quantities. In the next sequence of lemmas we give some bounds (lower and upper ones) on a_i's and b_j's.

Lemma 1.1

For any $s = 1, \ldots, h$ *we have*

$$b_s \frac{N_s}{\kappa - N_s} \leq a_s \leq b_1 \frac{N_s}{\kappa - N_s}; \tag{1}$$

Moreover, if $i = 0, \ldots, s-1$, *then*

$$\frac{N_s - N_i}{\kappa - N_i} b_s \leq a_s - a_i \leq \frac{\kappa}{\kappa - N_i} \frac{N_s - N_i}{\kappa - N_s} b_1. \tag{2}$$

Lemma 1.2

For any $t = 1, \ldots, h$,

$$\frac{1 - a_{t-1} M_{t-1}}{\kappa - n + 2 + M_{t-1}} \leq b_t \leq \frac{1 - a_1 M_{t-1}}{\kappa - n + 2 + M_{t-1}}, \tag{3}$$

and

$$\frac{(\kappa - N_h) a_h + M_{t,h} a_t}{\kappa - n + 2 + M_{t-1}} \leq b_t \leq \frac{\kappa - N_h + M_{t,h}}{\kappa - n + 2 + M_{t-1}} a_h. \tag{4}$$

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Lemma 1.3

For any $t = 1, \ldots, h$,

$$b_t \geq \frac{1}{\bar{\kappa}_t} \left(1 - \sum_{i=1}^{t-1} \frac{m_i N_i}{\bar{\mu}_i} \right). \tag{5}$$

Lemma 1.4

For any $s = 1, \ldots, h$, *we have*

$$a_s \leq \frac{1}{\bar{\mu}_s} \left(N_s - a_1 \bar{e}_s \right), \tag{6}$$

where $\bar{e}_s = \sum_{j=1}^{s} n_j M_{j-1}$

Clearly, (6) is an improvement of the right hand side of (1).

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Lemma 1.5

For any $s = 1, \ldots, h$,

$$a_s \geq \frac{N_s}{\bar{\mu}_s} \left(1 - \sum_{j=1}^{s} \frac{n_j}{N_s} \left(\sum_{i=1}^{j-1} \frac{m_i N_i}{\bar{\mu}_i} + \frac{M_{j-1}}{\bar{\kappa}_j} \right) \right). \tag{7}$$

We shall now refine the upper bound for a_s (see (1)

Lemma 1.6

For any $t = 1, \ldots, h$ *we have*

$$b_t \leq \frac{1}{\bar{\kappa}_t}\left(1 - \sum_{i=1}^{t-1} \frac{m_i N_i}{\bar{\mu}_i} + \sum_{i=1}^{t-1} \frac{m_i}{\bar{\mu}_i} \sum_{j=1}^{i} n_j \left(\sum_{k=1}^{j-1} \frac{m_k N_k}{\bar{\mu}_k} + \frac{M_{j-1}}{\bar{\kappa}_j}\right)\right). \qquad (8)$$

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Theorem 1.7

For any s*, with* $1 \leq s \leq h$*, we have*

$$\begin{aligned} a_s \quad \leq \quad & \frac{N_s}{\bar{\mu}_s}\left(1 - \sum_{j=1}^{s} \frac{n_j}{N_s}\left(\sum_{i=1}^{j-1} \frac{m_i N_i}{\bar{\mu}_i} + \frac{M_{j-1}}{\bar{\kappa}_j}\right) + \right. \qquad (9) \\ & \sum_{j=1}^{s} \frac{n_j}{N_s} \sum_{i=1}^{j-1} \frac{m_i}{\bar{\mu}_i} \sum_{k=1}^{i} n_k \left(\sum_{\ell=1}^{k-1} \frac{m_\ell N_\ell}{\bar{\mu}_\ell} + \frac{M_{k-1}}{\bar{\kappa}_k}\right) + \\ & \left.\sum_{j=1}^{s} \frac{n_j M_{j-1}}{N_s \bar{\kappa}_j} \sum_{i=1}^{j-1} \frac{m_i}{\bar{\mu}_i}\left(N_i - \sum_{k=1}^{i} n_k \left(\sum_{\ell=1}^{k-1} \frac{m_\ell N_\ell}{\bar{\mu}_\ell} + \frac{M_{k-1}}{\bar{\kappa}_k}\right)\right)\right). \end{aligned}$$

The results from the above lemmas can be summarized as follows:

Theorem 1.8

For any s, t, with $1 \leq s, t \leq h$, let

$$\alpha_s = \frac{N_s}{\bar{\mu}_s}\left(1 - \sum_{j=1}^{s} \frac{n_j}{N_s}\left(\sum_{i=1}^{j-1} \frac{m_i N_i}{\bar{\mu}_i} + \frac{M_{j-1}}{\bar{\kappa}_j}\right)\right)$$

and

$$\beta_t = \frac{1}{\bar{\kappa}_t}\left(1 - \sum_{i=1}^{t-1} \frac{m_i N_i}{\bar{\mu}_i}\right).$$

Then

$$\alpha_s \leq a_s \leq \alpha_s + \frac{N_s}{\bar{\mu}_s}\left(\sum_{j=1}^{s} \frac{n_j}{N_s} \sum_{i=1}^{j-1} \frac{m_i}{\bar{\mu}_i} \sum_{k=1}^{i} n_k \left(\sum_{\ell=1}^{k-1} \frac{m_\ell N_\ell}{\bar{\mu}_\ell} + \frac{M_{k-1}}{\bar{\kappa}_k}\right) + \sum_{j=1}^{s} \frac{n_j M_{j-1}}{N_s \bar{\kappa}_j} \sum_{i=1}^{j-1} \frac{m_i}{\bar{\mu}_i}\left(N_i - \sum_{k=1}^{i} n_k \left(\sum_{\ell=1}^{k-1} \frac{m_\ell N_\ell}{\bar{\mu}_\ell} + \frac{M_{k-1}}{\bar{\kappa}_k}\right)\right)\right).$$

Some bounds on the $Q-$index of an NSG

In this section we will prove some bounds on the $Q-$index of NSGs. We start with lower ones.

Proposition 2.1

If G is a connected NSG, then

$$\kappa \geq \max_{1 \leq k \leq h} \frac{1}{2}[2d_k + \bar{d}_k - 1 + \sqrt{(2d_k + \bar{d}_k - 1)^2 - 8(d_h - 1)d_k}]. \tag{10}$$

In particular, for $k = h$ and $k = 1$, we get the following corollary.

Corollary 2.2

If G is a connected NSG, then

$$\kappa \geq \frac{1}{2}[3N_h - 2 + m_h + \sqrt{(N_h + m_h - 2)^2 + 4m_h n_h}] \tag{11}$$

and

$$\kappa \geq \frac{1}{2}[2n_1 + n - 2 + \sqrt{(n-2)^2 + 4n_1(n_1 + M_h - N_h)}]. \tag{12}$$

Lower bounds

Proposition 2.3

If G is a connected NSG, then

$$\kappa \geq \frac{1}{2}\left[\frac{\sum_{i=1}^{h} n_i \bar{d}_i}{N_h} + N_h - 1 + t + \sqrt{\left(\frac{\sum_{i=1}^{h} n_i \bar{d}_i}{N_h} + N_h - 1 - t\right)^2 + 4\hat{e}_h^*}\right],$$

where

$$t = \frac{\sum_{i=1}^{h} m_i N_i^3}{\sum_{i=1}^{h} m_i N_i^2} \quad \text{and} \quad \hat{e}_h^* = \sum_{i=1}^{h} \frac{N_i}{N_h} \hat{e}_i \,.$$

Demonstração.

Let $\mathbf{y} = (y_1, \ldots, y_n)^T$ be a vector whose components are indexed by the vertices of G, and let $y_u = N_i$ if $u \in U_i$, for some $i \in \{1, \ldots, h\}$, or, otherwise, $y_v = q = \kappa - t$, for some t if $v \in V_j$ for some $j \in \{1, \ldots, f\}$. Substituting y into the Rayleigh quotient we obtain

$$\kappa \geq \frac{2\sum_{i=1}^{h} m_i N_i^2 q + 2\binom{N_h}{2} q^2 + \sum_{i=1}^{h} m_i d_i N_i^2 + \sum_{i=1}^{h} n_i \bar{d}_i q^2}{\sum_{i=1}^{h} m_i N_i^2 + N_h q^2}.$$

Since $q = \kappa - t$, we get

$$N_h q^3 + \left[N_h t - 2\binom{N_h}{2} - \sum_{i=1}^{h} n_i \bar{d}_i \right] q^2 - \sum_{i=1}^{h} m_i N_i^2 q \geq \sum_{i=1}^{h} m_i N_i^3 - t \sum_{i=1}^{h} m_i N_i^2 .$$

Choosing $t = \dfrac{\sum_{i=1}^{h} m_i N_i^3}{\sum_{i=1}^{h} m_i N_i^2}$ and taking into account that $N_1 \leq t \leq N_h$, we immediately get a quadratic inequality in q and the proof is concluded. $\square$

Upper bounds

Proposition 2.4

If G is a connected NSG, then

$$q \leq \frac{1}{2}[2N_h + n - 2 + \sqrt{(n-2)^2 + 4e_h}], \tag{13}$$

where $e_h = \sum_{i=1}^{h} m_s N_s$.

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Proposition 2.5

If G is a connected NSG, then

$$q \leq \frac{1}{2}[2N_h + n - 2 + \sqrt{(n-2)^2 + 4e'_h}], \tag{14}$$

where

$$e'_h = e_h - n_1[\frac{M_h \overline{e}_h}{n(2n-2-n_1)} + \frac{n_1 \sum_{s=1}^{h} m_s \overline{e}_s}{n(2n-2-n_1)}]$$

Proposition 2.6

If G is a connected NSG, then

$$q \leq \frac{1}{2}[2N_h + n' - 2 + \sqrt{(n' - 2)^2 + 4e'_h}], \tag{15}$$

where

$$n' = n - \frac{n_1 \overline{e}_h}{n(2n-2-n_1)}, \qquad e'_h = e_h - \frac{n_1 \sum_{s=1}^{h} m_s \bar{e}_s}{n(2n-2-n_1)}$$

Numerical examples

Example

We have $\nu = 20$, and assume that $\epsilon = 100$ and $N_h = 12$. There are 125 such NSGs, or $0, 1, 9, 30, 62, 22, 1, 0$ ones, for each $h = 1, 2, 3, 4, 5, 6, 7, 8$, respectively. In particular, for $h = 4$, we will take a sample graph (so one out of 30) with the following parameters:

$$m = (4, 2, 1, 1) \quad \text{and} \quad n = (2, 1, 5, 4)\,.$$

The exact value of the Q-index and the corresponding (lower and upper) bounds (together with errors) are given in the following table:

Prop. 2.2	Prop.2.3	κ	Prop. 2.4	Prop.2.5	Prop. 2.6
24.0000 −10.5 %	26.0594 −2.80 %	26.8105 0	31.3072 16.8 %	31.3538 16.9 %	31.7238 18.3 %

Example

The NSGs given here will be derived from the NSG considered in the previous example. We first multiply each of its (basic) parameters by 10, 100, and 1000, respectively. Then we get:

1. an NSG with $m = (40, 20, 10, 10)$, $n = (20, 10, 50, 40)$:

Prop. 2.2	Prop.2.3	κ	Prop. 2.4	Prop.2.5	Prop. 2.6
256.774 −9.88%	277.454 −2.62%	284.920 0	329.782 16.7%	330.250 15.9%	333.896 17.2%

2. an NSG with $m = (400, 200, 100, 100)$, $n = (200, 100, 500, 400)$

Prop. 2.2	Prop.2.3	κ	Prop. 2.4	Prop.2.5	Prop. 2.6
2584.66 −9.82%	2791.51 −2.60%	2866.13 0	3314.63 15.6%	3319.32 15.8%	3355.72 17.1%

Example

1. an NSG with $m = (4000, 2000, 1000, 1000)$, $n = (2000, 1000, 5000, 4000)$

Prop. 2.2	Prop.2.3	κ	Prop. 2.4	Prop.2.5	Prop. 2.6
25863.6 -9.81%	27932.1 -2.60%	28678.3 0	33163.1 15.6%	33210.0 15.8%	33574.0 17.1%

The following sample graphs are obtained by multiplying only one of the parameters from the NSG of Example 5.1 by 10000. Then we have:

2. an NSG with $m = (40000, 2, 1, 1)$, $n = (2, 1, 5, 4)$.

Prop. 2.2	Prop.2.3	κ	Prop. 2.4	Prop.2.5	Prop. 2.6
40018.0 $-2.5 \cdot 10^{-6}\%$	6692.83 -83.3%	40018.0 0	40024.0 0.015%	40024.0 0.015%	40028.0 0.025%

Example

1. an NSG with $m = (4, 20000, 1, 1)$, $n = (2, 1, 5, 4)$.

Prop. 2.2	Prop.2.3	κ	Prop. 2.4	Prop.2.5	Prop. 2.6
20020.0 $-5.6 \cdot 10^{-3}\%$	5027.32 -74.9%	20021.1 0	20028.4 0.037%	20028.4 0.037%	20031.0 0.049%

2. an NSG with $m = (4, 2, 10000, 1)$, $n = (2, 1, 5, 4)$.

Prop. 2.2	Prop.2.3	κ	Prop. 2.4	Prop.2.5	Prop. 2.6
10027.0 -0.022%	6698.81 -33.2%	10029.2 0	10036.5 0.073%	10036.5 0.073%	10037.0 0.078%

Example

-an NSG with $m = (4, 2, 1, 10000)$, $n = (2, 1, 5, 4)$.

Prop. 2.2	Prop.2.3	κ	Prop. 2.4	Prop.2.5	Prop. 2.6
10034.0 -0.021 %	10035.8 $-2.8 \cdot 10^{-3}$ %	10036.1 0	10041.0 0.049 %	10041.0 0.049 %	10041.0 0.049 %

- an NSG with $m = (4, 2, 1, 1)$, $n = (20000, 1, 5, 4)$.

Prop. 2.2	Prop.2.3	κ	Prop. 2.4	Prop.2.5	Prop. 2.
40020.0 -0.03 %	40034.0 $-1 \cdot 10^{-8}$ %	40034.0 0	40034.0 $1.5 \cdot 10^{-5}$ %	40034.0 $1.5 \cdot 10^{-5}$ %	40034. $2.3 \cdot 10^{-5}$

Example

-an NSG with $m = (4, 2, 1, 1)$, $n = (2, 10000, 5, 4)$.

Prop. 2.2	Prop.2.3	κ	Prop. 2.4	Prop.2.5	Prop. 2.6
20022.0	20028.0	20028.0	20032.0	20032.0	20032.0
-0.029 %	$-1.6 \cdot 10^{-8}$ %	0	0.02 %	0.02%	0.02 %

- an NSG with $m = (4, 2, 1, 1)$, $n = (2, 1, 50000, 4)$.

Prop. 2.2	Prop.2.3	κ	Prop. 2.4	Prop.2.5	Prop.
100014.0	100016.0	100016.0	100022.0	100022.0	10002
$-2 \cdot 10^{-3}$ %	$-4.7 \cdot 10^{-11}$ %	0	$6 \cdot 10^{-3}$ %	$6 \cdot 10^{-3}$ %	$6 \cdot 10$

Example

- an NSG with $m = (4, 2, 1, 1)$, $n = (2, 1, 5, 40000)$.

Prop. 2.2	Prop.2.3	κ	Prop. 2.4	Prop.2.5	Prop
80016.0 $-7 \cdot 10^{-7}$ %	80016.0 $-1 \cdot 10^{-10}$ %	80016.0 0	80023.0 $8.7 \cdot 10^{-3}$ %	80023.0 $8.7 \cdot 10^{-3}$ %	800 $8.7 \cdot 1$