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Spectral Characterizations of the Lovász Number and the Delsarte Number of a Graph

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Abstract. This paper gives spectral characterizations of two closely related graph functions: the Lovász number ϑ and a generalization ϑ^1 of Delsarte's linear programming bound. There are many known characterizations of the Lovász number ϑ, and each one corresponds to a similar characterization of ϑ^1 obtained by extremizing over a larger or smaller class of objects.

The spectral characterizations of ϑ and ϑ^1 given here involve the largest eigenvalue of a type of weighted Laplacian that Fan Chung introduced.

Keywords: graph Laplacian, Delsarte linear programming bound, Lovász number

1. Introduction

Many graph functions, such as the chromatic number and the clique number, have been devised to encode information about the geometry, topology, or combinatorics of a graph. Here we study two graph functions that have been around for a few decades and that are closely related to each other. One, known as the Lovász number, was first introduced by Lovász [6] in 1979 as an upper bound for a quantity called the Shannon capacity; the other, introduced by McEliece, Rodemich, Rumsey [8], and Schrijver [9], is a generalization of Delsarte's linear programming upper bound for the independence number. In his original paper, Lovász gave several different characterizations of his graph invariant; still others were developed later. The second invariant considered here also has many different characterizations; in fact, each is similar to a corresponding characterization of the Lovász number, except that it is obtained by extremizing over a larger or smaller class of objects (see the Table of characterizations in §3). Besides its famous application to the Shannon capacity of a graph, much of the interest in the Lovász number results from its diverse characterizations, according to Knuth [5].

This paper establishes for each of the two graph invariants yet another characterization, involving the spectrum of a type of weighted Laplacian introduced by Fan Chung [1]. She defined a spectral graph invariant in order to bound the chromatic number from below, and we show that it is exactly the same graph invariant considered by McEliece, Rodemich, Rumsey, and Schrijver. This work was motivated by a study of Chung's spectral graph invariant and an attempt to relate it to other known graph invariants.

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This paper is arranged as follows: In §2, we define basic terms. In §3, we introduce the two graph invariants and summarize their known characterizations. In §4, we define the weighted Laplacian and state our main theorem. After establishing some properties of weighted Laplacians in §§5–6, we prove the theorem in §§7-8.

2. Preliminary definitions and notation

In this paper, G is a graph on n vertices. The vertices of G are labelled $1, 2, \ldots, n$. The notation $i \sim j$ indicates that vertex i is adjacent to vertex j; the notation $i \nsim j$ indicates either that $i = j$ or that i and j are distinct non-adjacent vertices. The graph $\bar{G}$ is the complement of G. The *clique number of* G, denoted by $\omega(G)$, is the size of a largest clique that is a subgraph of G. The *independence number of* G, denoted by $\alpha(G)$, is the size of a largest subset Y of the vertex set of G such that no two vertices in Y are adjacent. The independence number and the clique number are related by $\omega(G) = \alpha(\bar{G})$. The *chromatic number of* G, denoted by $\chi(G)$, is the smallest number of colors needed to color the vertices of G so that no two adjacent vertices have the same color.

We use the notation $\mathcal{S}_n$ to denote the set of real symmetric $n \times n$ matrices, and $\mathcal{S}_n^+$ to denote the set of real symmetric $n \times n$ matrices all of whose entries are non-negative. For any $A \in \mathcal{S}_n$, let $\Lambda(A)$ denote the largest eigenvalue of A. (This is not necessarily the largest in absolute value, since A may have a negative eigenvalue whose absolute value exceeds $\Lambda(A)$.) The smallest eigenvalue of A is $-\Lambda(-A)$. We use the notation Spec(A) to denote the set of eigenvalues. We say that a vector $v \in \mathbb{R}^n$ is *positive* if each of its components is a positive number. The Euclidean inner product of vectors $u, v \in \mathbb{R}^n$ is denoted by $u \cdot v$.

If N is some natural number, then a mapping $a : \{1, \ldots, n\} \to \mathbb{R}^N$ is called an *N-labelling* of the graph G on n vertices. We usually write a_j instead of $a(j)$. An N-labelling of G is called a *labelling with acute* (*resp. right*, *obtuse*) *angles* if $a_i \cdot a_j \geq 0$ (resp. $= 0, \leq 0$) for all $i \sim j$; it is called an *N-orthogonal labelling* if $a_i \cdot a_j = 0$ whenever i and j are distinct non-adjacent vertices in G; and it is called an *N-orthonormal labelling* if it is orthogonal and if $\|a_i\| = 1$ for each i.

3. Characterizations of ϑ and ϑ^1

In the late 1970's, Lovász [6] introduced a graph invariant, ϑ, as an upper bound for the Shannon capacity of a graph. He used it to determine the Shannon capacity of the five cycle and went on to give many alternative characterizations of ϑ. He also showed that $\omega(G) \leq \vartheta(\bar{G}) \leq \chi(G)$, inspiring the title of Knuth's survey [5].

Building on the work of Lovász, the authors McEliece, Rodemich, and Rumsey [8] introduced a slightly different function that was a bound on the independence number of a graph. They showed that for a certain class of graphs that arises naturally in information theory, their function was identical to the so-called Delsarte linear programming bound. They called their function one of two "Lovász bounds" (their other "Lovász bound" being ϑ). For the sake of uniqueness of names we will call it the "Delsarte number" and denote it by ϑ^1. McEliece, Rodemich, and Rumsey show in [8] that $\vartheta^1(G) \geq \alpha(G)$ or, equivalently, $\vartheta^1(\bar{G}) \geq \omega(G)$.

Schrijver [9] considered the same function and found some of the same results that are contained in [8]. The work of Schrijver also built upon that of Lovász but was independent of that of McEliece, Rodemich, and Rumsey.

Below, we summarize the previously known characterizations of $\vartheta(\bar{G})$ and $\vartheta^1(\bar{G})$ for a graph G having at least one edge. Lovász gave the first five characterizations of ϑ and proved their equivalence in his first paper on the topic [6]. The sixth and seventh characterizations of ϑ appear in [9] and [2], respectively. Definitions of ϑ^1 were given independently in [9] (second and third characterizations below) and [8] (sixth characterization). To prove that the first, fourth, fifth, and seventh characterizations of ϑ^1 below are equivalent to the others, one can mimic the proofs establishing the corresponding characterizations of ϑ. We omit the straightforward details; a readable and thorough reference for proofs about ϑ is Knuth's survey [5].

Table of characterizations of ϑ and ϑ^1 ([2, 6, 8, 9])

1. $\vartheta^{(1)}(\bar{G}) = \min\{\max_i \frac{1}{(b\cdot a_i)^2} : \|b\| = 1, a \in \mathsf{A}^{(1)}\}$

$$\begin{aligned}\mathsf{A}^1 &= \{a : a = \text{labelling of } G \text{ with obtuse angles}, \|a_i\| = 1 \text{ for all } i\}\\ \mathsf{A} &= \{a : a = \text{labelling of } G \text{ with right angles}, \|a_i\| = 1 \text{ for all } i\}\\ &= \{a : a = \text{o.n. labelling of } \bar{G}\}\end{aligned}$$

2. $\vartheta^{(1)}(\bar{G}) = \min\{\Lambda(A) : A \in \mathcal{A}^{(1)}\}$

$$\begin{aligned}\mathcal{A}^1 &= \{A = (a_{ij}) \in \mathcal{S}_n : a_{ij} \geq 1 \text{ whenever } i = j \text{ or } i \sim j\}\\ \mathcal{A} &= \{A = (a_{ij}) \in \mathcal{S}_n : a_{ij} = 1 \text{ whenever } i = j \text{ or } i \sim j\}.\end{aligned}$$

3. $\vartheta^{(1)}(\bar{G}) = \max_{D\in\mathcal{D}^{(1)}} \sum_{i,j=1}^n d_{ij} = \max_{a\in\mathsf{B}^{(1)}} \sum_{i,j} a_i \cdot a_j = \max_{a\in\mathsf{B}^{(1)}} \|S^{(a)}\|^2$

$$\begin{aligned}\mathcal{D}^1 &= \{D \in \mathcal{S}_n^+ : \mathrm{Tr}(D) = 1, D \text{ positive semidefinite}, d_{ij} > 0 \text{ only if } i \sim j \text{ or } i = j\}\\ \mathcal{D} &= \{D \in \mathcal{S}_n : \mathrm{Tr}(D) = 1, D \text{ positive semidefinite}, d_{ij} \neq 0 \text{ only if } i \sim j \text{ or } i = j\}\\ \mathsf{B}^1 &= \left\{a : a = \text{orthogonal labelling of } G \text{ with acute angles}, \sum_{j=1}^n \|a_j\|^2 = 1\right\}\\ \mathsf{B} &= \left\{a : a = \text{orthogonal labelling of } G, \sum_{j=1}^n \|a_j\|^2 = 1\right\}, S^{(a)} = \sum_j a_j\end{aligned}$$

4. $\vartheta^{(1)}(\bar{G}) = \max\{\sum_{i=1}^n x_i : x \in \mathsf{C}^{(1)}\}$

$$\begin{aligned}\mathsf{C}^1 &= \{((d\cdot a_i)^2) \in \mathbb{R}^n : \|d\|_{\mathbb{R}^N} = 1, a = N\text{-orthonormal labelling of } G \text{ with acute angles}\}\\ \mathsf{C} &= \{((d\cdot a_i)^2) \in \mathbb{R}^n : \|d\|_{\mathbb{R}^N} = 1, a = N\text{-orthonormal labelling of } G\}.\end{aligned}$$

5. $\vartheta^{(1)}(\bar{G}) = 1 + \max\{\frac{\Lambda(B)}{\Lambda(-B)} : B \in \mathcal{B}^{(1)}\}$

$$\mathcal{B}^1 = \{0 \neq B = (b_{ij}) \in \mathcal{S}_n^+ : b_{ij} \neq 0 \text{ only if } i \sim j\}$$
$$\mathcal{B} = \{0 \neq B = (b_{ij}) \in \mathcal{S}_n : b_{ij} \neq 0 \text{ only if } i \sim j\}$$

6. $\vartheta^{(1)}(\bar{G}) = \min\{1/\lambda(A) : A \in \Omega^{(1)}\}$

$$\lambda(A) = \min\left\{x^T A x : x \in \mathbb{R}^n, \sum_i x_i = 1\right\}$$
$$\Omega^1 = \{A = (a_{ij}) \in \mathcal{S}_n : a_{ii} = 1, a_{ij} \leq 0 \text{ if } i \sim j, A \text{ positive semidefinite }\}$$
$$\Omega = \{A = (a_{ij}) \in \mathcal{S}_n : a_{ii} = 1, a_{ij} = 0 \text{ if } i \sim j, A \text{ positive semidefinite }\}.$$

7. $\vartheta^{(1)}(\bar{G}) = \max\{\Lambda(C) : C \in \mathcal{C}^{(1)}\}$

$$\mathcal{C}^1 = \{C \in \mathcal{S}_n^+ : C \text{ positive semidefinite}, c_{ij} - \delta_{ij} \neq 0 \text{ only if } i \sim j\}$$
$$\mathcal{C} = \{C \in \mathcal{S}_n : C \text{ positive semidefinite}, c_{ij} - \delta_{ij} \neq 0 \text{ only if } i \sim j\}$$

Warning. Some sources call this quantity $\vartheta(G)$ instead of $\vartheta(\bar{G})$. In [8], $\vartheta(G)$ is denoted $\vartheta_L(\bar{G})$. Our notation here is consistent with that of Knuth's survey [5] and that of some work by Lovász and others [2], but not with that of Lovász's first paper on the subject [6].

Comparing the sets over which we extremize in order to obtain either $\vartheta^1(\bar{G})$ or $\vartheta(\bar{G})$, we see immediately that $\vartheta^1(\bar{G}) \leq \vartheta(\bar{G})$. This leads to an "extended sandwich"

$$\omega(G) \leq \vartheta^1(\bar{G}) \leq \vartheta(\bar{G}) \leq \chi(G).$$

In [9], Schrijver also cites M.R. Best's example of a graph $\bar{G}$ for which $\vartheta(\bar{G}) \neq \vartheta^1(\bar{G})$. The vertices of the graph $\bar{G}$ are all vectors in $\{0, 1\}^6$ and two such vertices are adjacent if and only if they differ in at most three of the six coordinate places.

4. Weighted graph Laplacian

Fan Chung recently introduced a weighted graph Laplacian [1] that turns out to yield yet another pair of characterizations of ϑ and ϑ^1. We define the Laplacian and state the new characterizations of ϑ and ϑ^1 in this section, deferring the proofs until later.

Let G be a graph with its vertices labelled from 1 to n. Assume for now that G has at least one edge. In the definition below, $\mathcal{W}^1$ is a class of weight matrices that Chung considered, while $\mathcal{W}$ is a larger class introduced in this paper.

Definition 1 If $W = (w_{ij}) \in \mathcal{S}_n$ then let

$$w_i = \sum_{j=1}^{n} w_{ij}.$$

Let

$$\begin{aligned}\mathcal{W}^1 &= \{0 \neq (w_{ij}) \in \mathcal{S}_n^+ : w_{ij} > 0 \text{ only if } i \sim j\} \text{ and}\\ \mathcal{W} &= \{0 \neq (w_{ij}) \in \mathcal{S}_n : w_{ij} \neq 0 \text{ only if } i \sim j;\ w_i \geq 0\,\forall i;\\ &\qquad w_i = 0 \text{ only if } w_{ij} = 0\,\forall j\}.\end{aligned}$$

Clearly $\mathcal{W}^1 \subseteq \mathcal{W}$. Elements of $\mathcal{W}$ are called *weight matrices for G*. The sets $\mathcal{W}$ and $\mathcal{W}^1$ are nonempty as long as G has at least one edge.

Definition 2 We define the *weighted Laplacian* of G with weight matrix $W \in \mathcal{W}^1$ to be the $n \times n$ matrix L_W with entries

$$(L_W)_{ij} = \begin{cases} 1 & \text{if } i = j \text{ and } w_i \neq 0\\ -\dfrac{w_{ij}}{\sqrt{w_i w_j}} & \text{if } i \sim j \text{ and } w_i w_j \neq 0\\ 0 & \text{otherwise.}\end{cases}$$

Observe that $L_W(\sqrt{w_1}, \ldots, \sqrt{w_n})^{\mathrm{T}} = 0$. Also, if W is in the smaller set $\mathcal{W}^1$ then L_W is positive semidefinite [1]. If W is in $\mathcal{W}$ but not in $\mathcal{W}^1$, then (unlike most discrete and continuous operators that go by the name "Laplacian") L_W is not necessarily positive semidefinite.

Our main result is the following:

Theorem 1 *If G has at least one edge then*

$$\vartheta(\bar{G}) = 1 + \max\left\{\frac{1}{\Lambda(L_W) - 1} : W \in \mathcal{W}, L_W \text{ positive semidefinite}\right\} \tag{1}$$

and

$$\vartheta^1(\bar{G}) = 1 + \max\left\{\frac{1}{\Lambda(L_W) - 1} : W \in \mathcal{W}^1\right\} \tag{2}$$

where $\Lambda(L_W)$ is the largest eigenvalue of L_W.

We will prove this theorem in Sections 7 and 8.

5. Properties of graph invariant σ

Using the notation that Fan Chung introduced in [1], we have

Definition 3 The graph invariant

$$\sigma(G) \stackrel{\text{def}}{=} 1 + \max\left\{\frac{1}{\Lambda(L_W) - 1} : W \in \mathcal{W}^1\right\}$$

if G has at least one edge. If G has no edges, then define $\sigma(G) = 1$.

Our first goal will be to establish the relationship between σ of a graph and σ of its various connected components. This will result in a convenient set of criteria to determine when a given graph function is identically equal to σ.

Lemma 1 *Let H be a subgraph of G. Then*

$$\sigma(H) \le \sigma(G).$$

Furthermore, if H is obtained from G by removing isolated vertices then $\sigma(H) = \sigma(G)$.

Evaluating σ for a subgraph is equivalent to optimizing over a smaller set of matrices. We omit the straightforward details involved in proving the lemma.

Lemma 2 *If G is the disjoint union of graphs G_1 and G_2, then*

$$\sigma(G) = \max\{\sigma(G_1), \sigma(G_2)\}.$$

Proof: If either G_1 or G_2 contains no edges then the statement is a consequence of Lemma 1. If each G_i contains an edge them Lemma 1 still implies $\sigma(G_i) \le \sigma(G)$ for both $i = 1, 2$. To show that equality holds for either $i = 1$ or $i = 2$, consider the matrix K that achieves the max in the definition of $\sigma(G)$. Then L is formed from blocks L_1 and L_2 corresponding to Laplacians of G_1 and G_2, respectively. By renumbering we may assume that $\Lambda(L) = \Lambda(L_1)$, which implies

$$\sigma(G) = 1 + \frac{1}{\Lambda(L) - 1} = 1 + \frac{1}{\Lambda(L_1) - 1} \le \sigma(G_1) \le \sigma(G). \qquad \square$$

Remark Using the preceding lemmas, we can compute $\sigma(G)$ for any graph by computing $\sigma(G_i)$ for each connected component G_i. Furthermore, we have the following immediate useful consequence of Lemma 2:

Lemma 3 *Let $\tilde{\sigma}$ be a graph function. If*
(H1) $\tilde{\sigma}(G) = \sigma(G)$ whenever G is connected; and
(H2) $\tilde{\sigma}(G) = \max\{\tilde{\sigma}(G_1), \tilde{\sigma}(G_2)\}$ whenever G is the disjoint union of G_1 and G_2,
then $\sigma(G) = \tilde{\sigma}(G)$ for all G.

6. Weight matrices and induced Laplacians

The following lemma allows us to compute σ using a more convenient class of weight matrices.

Lemma 4 *Assume that G is connected. Then*

$$\sup_{W\in\mathcal{W}^1}\frac{1}{\Lambda(L_W)-1}=\sup_{W\in\mathcal{W}^\circ}\frac{1}{\Lambda(L_W)-1} \tag{3}$$

where $\mathcal{W}^1=\{0\neq(w_{ij})\in\mathcal{S}_n^+ : w_{ij}>0$ *only if* $i\sim j\}$ *and* $\mathcal{W}^\circ=\{0\neq(w_{ij})\in\mathcal{S}_n^+ : w_{ij}>0$ *if and only if* $i\sim j\}$.

Proof: This proof is essentially a continuity argument. If we interpret the condition $w_i=0$ as a "pretense" that vertex i is isolated, then we will approximate an isolated vertex by a vertex connected to certain others but with very small weights on those connecting edges. Similarly, if $w_{ij}=0$ corresponds to pretending that the i,j edge is not there, then we will approximate that situation by an i,j edge with very small weight.

Since $\mathcal{W}^\circ\subseteq\mathcal{W}^1$, (3) is true if we replace "=" by "≥". To show the reverse inequality, it suffices to show that for any $W\in\mathcal{W}^1$ there are matrices in $\mathcal{W}^\circ$ whose maximum eigenvalues are arbitrarily close to $\Lambda(W)$. We will do this in two steps, addressing first the issue of positive row sums $w_i=\sum_j w_{ij}$ and then the question of positive weights on all edges of G.

Let $W\in\mathcal{W}^1$ and assume that $w_i=0$ for $i=k+1,\dots,n$ and $w_i>0$ for $i=1,\dots,k$. Then we can write W in the block form

$$W=\begin{pmatrix}A & 0\\ 0 & 0\end{pmatrix}$$

where $A\in\mathcal{S}_k^+$ and $a_i=\sum_{j=1}^k a_{ij}$ is strictly positive for each $i=1,\dots,k$.

For any $\epsilon>0$, let

$$W'_\epsilon=\begin{pmatrix}A & B_\epsilon\\ B_\epsilon^{\mathrm{T}} & 0\end{pmatrix}$$

where the entries of B_ϵ are defined to be ϵ if $i\sim j$ and 0 otherwise. Since G is connected, B is not identically zero. Then each row sum of W'_ϵ is positive and there are positive integers c_i independent of ϵ such that

$$(W'_\epsilon)_i=\begin{cases}a_i+c_i\epsilon & i=1,\dots,k\\ c_i\epsilon & i=k+1,\dots,n.\end{cases}$$

Since $a_i>0$, a straightforward computation of $L_{W'_\epsilon}$ shows that

$$L_W=\begin{pmatrix}L_A & 0\\ 0 & 0\end{pmatrix}\quad\text{and}$$

$$\lim_{\epsilon\to0}L_{W'_\epsilon}=\begin{pmatrix}L_A & 0\\ 0 & I\end{pmatrix}$$

where the convergence is with respect to the Euclidean $\mathbb{R}^{n^2}$ norm, for example. Since Λ is a continuous function,

$$\lim_{\epsilon\to 0} \Lambda(L_{W'_\epsilon}) = \Lambda\left(\lim_{\epsilon\to 0} L_{W'_\epsilon}\right) = \max\{\Lambda(L_W), 1\} = \Lambda(L_W).$$

We remark that W'_ϵ is not in the class $\mathcal{W}^\circ$, but as in the next step it may be approximated by matrices in $\mathcal{W}^\circ$.

To address the issue of positive weights on all edges of G, we proceed in a similar way. Starting from any $W = (w_{ij}) \in \mathcal{W}$ with positive row sums but not necessarily positive weights on all edges of G, define

$$(W_\epsilon)_{ij} = \begin{cases} \epsilon & i \sim j \text{ and } w_{ij} = 0 \\ w_{ij} & \text{otherwise.} \end{cases}$$

Note that $W_\epsilon \in \mathcal{W}^\circ$. Also, $\lim_{\epsilon\to 0} L_{W_\epsilon} = L_W$ and hence $\lim_{\epsilon\to 0} \Lambda(L_{W_\epsilon}) = \Lambda(L_W)$. The two approximations from this proof, used in conjunction, show that the supremum of $1/(\Lambda(L_W) - 1)$ can be approached through Laplacians with weight matrices in the subclass $\mathcal{W}^\circ$. □

The next proposition characterizes those matrices that occur as Laplacians of a given graph.

Proposition 1 *Let G be a graph with no isolated vertices. Let*
$\mathcal{W}^\circ = \{0 \neq (w_{ij}) \in \mathcal{S}_n^+ : w_{ij} > 0$ *if and only if* $i \sim j\}$;
$\mathcal{B}^\circ = \{B \in \mathcal{W}^\circ : B$ *has a positive fixed vector* $\}$; *and*
$\mathcal{B}' = \{B \in \mathcal{S}_n : b_{ij} \neq 0$ *only if* $i \sim j$ *in* G, B *has a positive fixed vector* $\}$.

Then

$$\{L_W : W \in \mathcal{W}^\circ\} = \{I - B : B \in \mathcal{B}^\circ\}$$

and

$$\{L_W : W \in \mathcal{W} \text{ and } w_i > 0 \quad \text{for all } i\} = \{I - B : B \in \mathcal{B}'\}.$$

Proof: We will prove only the first conclusion; the proof of the second is similar. To show the inclusion $\{L_W : W \in \mathcal{W}^\circ\} \subseteq \{I - B : B \in \mathcal{B}^\circ\}$ we need to find a positive fixed vector of $I - L_W$. But as observed in the text following Definition 2, $(\sqrt{w_1}, \ldots, \sqrt{w_n})^{\mathrm{T}}$ is a null vector of L_W and it is positive if $W \in \mathcal{W}^\circ$. The remaining requirements for $I - L_W$ to be in $\mathcal{B}^\circ$ follow from the definitions of L_W and $\mathcal{W}^\circ$.

To show that $\{I - B : B \in \mathcal{B}^\circ\} \subseteq \{L_W : W \in \mathcal{W}^\circ\}$, let $B \in \mathcal{B}^\circ$. Let $v = (v_i)$ be a positive fixed vector of B, which exists by assumption. Define the $n \times n$ matrix $W = (w_{ij})$ by

$$w_{ij} = \begin{cases} v_i v_j b_{ij} & \text{if } i \sim j \\ 0 & \text{otherwise.} \end{cases}$$

Then $W \in \mathcal{W}^\circ$ and for each $i = 1, \ldots, n$,

$$w_i = \sum_j w_{ij} = v_i \sum_{j\sim i} v_j b_{ij} = v_i (Bv)_i = v_i^2.$$

Thus $v_i = \sqrt{w_i}$ since v_i is positive. By the definition of weighted Laplacians, whenever $i \sim j$ we have

$$(L_W)_{ij} = -\frac{w_{ij}}{\sqrt{w_i w_j}} = -\frac{v_i v_j b_{ij}}{v_i v_j} = -b_{ij} = (I - B)_{ij}.$$

Checking that $(L_W)_{ij} = (I - B)_{ij} = \delta_{ij}$ whenever $i \nsim j$, we see that $I - B = L_W$. $\square$

7. Characterizing ϑ^1 using Laplacians

Now we are ready to prove half of the main result:

Proof of (2) in Theorem 1 Using the the fifth characterization of $\vartheta^1(\bar{G})$ given in the Table in Section 3, we will show that

$$\sigma(G) = 1 + \sup_{B\in\mathcal{B}^1(G)} \frac{\Lambda(B)}{\Lambda(-B)} \tag{4}$$

where

$$\mathcal{B}^1(G) = \{0 \neq B = (b_{ij}) \in \mathcal{S}_n^+ : b_{ij} \neq 0 \text{ only if } i \sim j \text{ in } G\}.$$

First assume that G is connected and has at least one edge. By Lemma 4,

$$\sigma(G) = 1 + \sup_{\mathcal{W}^1} \frac{1}{\Lambda(L_W) - 1} = 1 + \sup_{\mathcal{W}^\circ} \frac{1}{\Lambda(L_W) - 1} = 1 + \sup_{\mathcal{W}^\circ} \frac{1}{\Lambda(L_W - I)}.$$

Using Proposition 1 we can write

$$\sigma(G) = 1 + \sup_{\mathcal{B}^\circ} \frac{1}{\Lambda(-B)}$$

where we recall that $\mathcal{B}^\circ = \{B = (b_{ij}) \in \mathcal{S}_n^+ : B$ has a positive fixed vector and $b_{ij} > 0$ if and only if $i \sim j\}$.

Furthermore, if $B \in \mathcal{S}_n^+$ satisfies $\Lambda(B) = 1$ and $b_{ij} > 0$ if and only if $i \sim j$, then the Perron-Frobenius Theorem implies that B has a positive eigenvector v. By the Perron-Frobenius Theorem, a positive eigenvector for a non-negative matrix must correspond to the largest eigenvalue. Therefore we can phrase our formula as

$$\sigma(G) = 1 + \sup\left\{\frac{1}{\Lambda(-B)} : B \in \mathcal{S}_n^+, \Lambda(B) = 1, b_{ij} > 0 \text{ if and only if } i \sim j\right\}. \tag{5}$$

All of the matrices $(b_{ij}) \in \mathcal{S}_n^+$ that satisfy $b_{ij} > 0$ if and only if $i \sim j$ have trace zero and hence a positive largest eigenvalue. Since for such matrices the expression $\Lambda(B)/\Lambda(-B)$ is unchanged if B is multiplied by a positive scalar, we may undo the normalization and write

$$\sigma(G) = 1 + \sup\left\{ \frac{\Lambda(B)}{\Lambda(-B)} : B \in \mathcal{S}_n^+, b_{ij} > 0 \text{ if and only if } i \sim j \right\}.$$

Finally, since Λ is a continuous function the supremum above is unchanged if we allow the matrices in question to have zeros corresponding to some, but not all, of the edges of G. Removing the "if" clause from the above expression and then explicitly excluding the zero matrix, we conclude that $\vartheta^1(\bar{G}) = \sigma(G)$ for connected graphs G.

Now suppose that G is the disjoint union of G_1 and G_2, where at least one G_i has an edge, and that vertices $1, \ldots, k$ of G are exactly the vertex set of G_1. We would like to establish hypothesis (H2) of Lemma 3.

If G_1 has an edge but G_2 does not, then the nonemptiness of $\mathcal{B}^1(G_1) \ni B$ and the fact that $\Lambda(-B), \Lambda(B) > 0$ imply that $\vartheta^1(\overline{G_1}) \geq 1 = \vartheta^1(\overline{G_2})$. Also, any $B \in \mathcal{B}^1(G)$ has the form

$$B = \begin{pmatrix} B_1 & 0 \\ 0 & 0 \end{pmatrix}$$

where $B_1 \in \mathcal{B}^+(G_1)$. Thus $\operatorname{Spec}(B) = \operatorname{Spec}(B_1) \cup \{0\}$. Since $\operatorname{Tr}(B) = 0$ and $B \neq 0$, zero is neither the largest nor the smallest eigenvalue of B. This means that $\Lambda(B)/\Lambda(-B) = \Lambda(B_1)/\Lambda(-B_1)$ and hence $\vartheta^1(\bar{G}) = \vartheta^1(\overline{G_1}) = \max\{\vartheta^1(\overline{G_1}), \vartheta^1(\overline{G_2})\}$.

If each G_i for $i = 1, 2$ has an edge then any $B \in \mathcal{B}^1(G)$ has the form

$$B = \begin{pmatrix} B_1 & 0 \\ 0 & B_2 \end{pmatrix}$$

where $B_i \in \mathcal{B}^+(G_i)$ is a square block. By writing B in this form we see that $\Lambda(B) = \max\{\Lambda(B_1), \Lambda(B_2)\}$ and $-\Lambda(-B) = \min\{-\Lambda(-B_1), -\Lambda(-B_2)\}$. Assume for convenience that $\Lambda(B) = \Lambda(B_1)$.

If $\Lambda(-B) = \Lambda(-B_1)$ then

$$1 + \frac{\Lambda(B)}{\Lambda(-B)} = 1 + \frac{\Lambda(B_1)}{\Lambda(-B_1)} \leq \max_{i=1,2}\{\vartheta^1(\overline{G_i})\}.$$

If, on the other hand, $\Lambda(-B) = \Lambda(-B_2)$ then $\Lambda(-B_2) \geq \Lambda(-B_1) > 0$ and hence

$$1 + \frac{\Lambda(B)}{\Lambda(-B)} = 1 + \frac{\Lambda(B_1)}{\Lambda(-B_2)} \leq 1 + \frac{\Lambda(B_1)}{\Lambda(-B_1)} \leq \max_{i=1,2} \vartheta^1(\overline{G_i}).$$

If we had $\Lambda(B) = \Lambda(B_2)$ to start with, then the same argument would show that again $1 + \Lambda(B)/\Lambda(-B) \leq \max_{i=1,2} \vartheta^1(\overline{G_i})$. Taking the supremum over $\mathcal{B}^1(G)$ we get

$$\vartheta^1(\bar{G}) \leq \max_{i=1,2} \vartheta^1(\overline{G_i}).$$

Since any $B_i \in \mathcal{B}^1(G_i)$ gives rise to an element $B \in \mathcal{B}^1(G)$ with $\Lambda(B_i)/\Lambda(-B_i) = \Lambda(B)/\Lambda(-B)$, we also have

$$\vartheta^1(\bar{G}) \geq \max_{i=1,2} \vartheta^1(\overline{G_i}).$$

Thus hypothesis (H2) holds in all cases. Since we have already proved hypothesis (H1), we now conclude from Lemma 3 that $\vartheta^1(\bar{G}) = \sigma(G)$. □

8. Characterizing ϑ using Laplacians

Lemma 5 *If $A \in \mathcal{S}_n$ and A_1 is a principal submatrix of A then $\Lambda(A_1) \leq \Lambda(A)$ and $-\Lambda(-A_1) \geq -\Lambda(-A)$.*

The lemma is part of the Interlacing Eigenvalues Theorem. Its proof relies on the variational characterizations of eigenvalues: that is, $\Lambda(A) = \sup_{v \neq 0} \frac{\langle Av, v\rangle}{\langle v, v\rangle}$ and $-\Lambda(-A) = \inf_{v \neq 0} \frac{\langle Av, v\rangle}{\langle v, v\rangle}$.

Proof of (1) in Theorem 1 Using the fifth characterization of $\vartheta(\bar{G})$ given in the Table in Section 3, we will show that the right side of (1) equals

$$1 + \sup_{B \in \mathcal{B}(G)} \frac{\Lambda(B)}{\Lambda(-B)}$$

where

$$\mathcal{B}(G) = \{0 \neq B = (b_{ij}) \in \mathcal{S}_n : b_{ij} \neq 0 \text{ only if } i \sim j \text{ in } G\}.$$

We first show that this is true if '$=$' is replaced by '$\geq$'. Let $W \in \mathcal{W}$ be such that $L = L_W$ is positive semidefinite. If some diagonal entry L_{ii} is zero then by the definition of the Laplacian the ith row and column must be identically zero. Without loss of generality assume that all zero rows are grouped at the bottom of L and that rows $1, \ldots, k$ are not identically zero. We can write

$$L = \begin{pmatrix} A & 0 \\ 0 & 0 \end{pmatrix}$$

where A is a positive semidefinite Laplacian matrix for the induced subgraph of G obtained by retaining vertices $1, \ldots, k$. By definition of k, $A_{ii} = 1$ for $i = 1, \ldots, k$. Define

$$L' = \begin{pmatrix} A & 0 \\ 0 & I_{n-k} \end{pmatrix}, \quad B = I_n - L'.$$

Since $\Lambda(L) > 1$, $\Lambda(L) = \Lambda(L')$. Since A is a positive semidefinite Laplacian, $\Lambda(-A) = 0$ and so $\Lambda(-L') = 0$. Furthermore, $B \in \mathcal{B}$ and $\Lambda(B) = 1 + \Lambda(-L') = 1$. Thus

$$\vartheta(\bar{G}) \geq 1 + \frac{\Lambda(B)}{\Lambda(-B)} = 1 + \frac{1}{\Lambda(L') - 1} = 1 + \frac{1}{\Lambda(L) - 1}.$$

Taking the supremum over all allowable W we see that $\vartheta(\bar{G})$ is greater than or equal to the right side of (1).

To show the reverse inequality, let $B \in \mathcal{B}$. Since we are using B to compute $\vartheta(\bar{G})$ via the fifth characterization in the Table of Section 3, we sacrifice no generality by assuming that $\Lambda(B) = 1$. Let $v = (v_i)$ be a vector such that $Bv = v$. Define the diagonal $n \times n$ matrix D by setting $D_{ii} = 1$ if $v_i \geq 0$ and $D_{ii} = -1$ if $v_i < 0$. Then $(Dv)_i = |v_i|$ for each i and $D^{-1} = D$. Notice that DBD^{-1} has the same eigenvalues as B and is still in $\mathcal{B}$. Thus by replacing B by DBD^{-1} and v by Dv if necessary, we may assume without loss of generality that v has all non-negative entries. We may also assume that v_i is strictly positive for all $i = 1, \ldots, k$ and that $v_i = 0$ for $i > k$.

Let $L = I - B$ and, as in the proof of Proposition 1, define weights

$$w_{ij} = \begin{cases} -v_i v_j L_{ij} & \text{if } i \sim j \\ 0 & \text{otherwise.} \end{cases}$$

Notice that $w_{ij} = 0$ if $i > k$ or $j > k$. If $i \leq k$ then

$$w_i = -v_i \sum_{j \sim i} v_j L_{ij} = -v_i(Lv - v_i L_{ii}) = (v_i)^2.$$

Using the fact that $v_i > 0$ for $i \leq k$, we can now check that $W = (w_{ij}) \in \mathcal{W}$. Let L_W be the Laplacian with weights (w_{ij}). If $i, j \leq k$ and $i \sim j$, then as in the proof of Proposition 1 we have $(L_W)_{ij} = L_{ij}$. Furthermore, if we write

$$L = \begin{pmatrix} A_1 & A_2 \\ A_2^T & A_3 \end{pmatrix} \quad \text{then} \quad L_W = \begin{pmatrix} A_1 & 0 \\ 0 & 0 \end{pmatrix}.$$

We claim that L_W is positive semidefinite: $-\Lambda(-L_W) = \min\{0, -\Lambda(-A_1)\}$ and $-\Lambda(-A_1) \geq -\Lambda(-L) = -\Lambda(B - I) = -\Lambda(B) + 1 = 0$. Therefore $-\Lambda(-L_W) = 0$. Finally, since $A_1 \neq I$ and $\mathrm{Tr}(A_1) = k$ we have $1 < \Lambda(L_W) = \Lambda(A_1) \leq \Lambda(L)$. Then $0 < \Lambda(L_W) - 1 \leq \Lambda(L - I) = \Lambda(-B)$ so that $(\Lambda(L_W) - 1)^{-1} \geq (\Lambda(-B))^{-1}$. Taking the supremum over all allowable B yields the result. $\square$

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