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On the bounds for the largest Laplacian eigenvalues of weighted graphs

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1. Introduction

A B S T R A C T

We consider weighted graphs, such as graphs where the edge weights are positive definite matrices. The Laplacian eigenvalues of a graph are the eigenvalues of the Laplacian matrix of a graph *G*. We obtain an upper bound for the largest Laplacian eigenvalue and we compare this bound with previously known bounds.

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We consider simple graphs, such as graphs which have no loops or parallel edges. Hence a graph G = (V, E) consists of a finite set of vertices, V, and a set of edges, E, each of whose elements is an unordered pair of distinct vertices. Generally V is taken as $V = \{1, 2, ..., n\}$.

A weighted graph is a graph each edge of which has been assigned to a square matrix called the weight of the edge. All the weight matrices are assumed to be of the same order and to be positive matrix. In this paper, by "weighted graph" we mean "a weighted graph with each of its edges bearing a positive definite matrix as weight", unless otherwise stated.

The following are the notations to be used in this paper. Let *G* be a weighted graph on *n* vertices. Denote by $w_{i,j}$ the positive definite weight matrix of order *p* of the edge *ij*, and assume that $w_{ij} = w_{ji}$. We write $i \sim j$ if vertices *i* and *j* are adjacent. Let $w_i = \sum_{j:j\sim i} w_{ij}$.

The Laplacian matrix of a graph *G* is defined as $L(G) = (l_{ij})$, where

 $l_{i,j} = \begin{cases} w_i; & \text{if } i = j, \\ -w_{ij}; & \text{if } i \sim j, \\ 0; & \text{otherwise.} \end{cases}$

Let λ_1 denote the largest eigenvalue of L(G). If V is the disjoint union of two nonempty sets V_1 and V_2 such that every vertex i in V_1 has the same $\lambda_1(w_i)$ and every vertex j in V_2 has the same $\lambda_1(w_j)$, then G is called a weight-semiregular graph. If $\lambda_1(w_i) = \lambda_1(w_j)$ in a weight semiregular graph, then G is called a weight-regular graph.

In the definitions above, the zero denotes the $p \times p$ zero matrix. Hence L(G) is a square matrix of order np.

Upper and lower bounds for the largest Laplacian eigenvalue for unweighted graphs have been investigated to a great extent in the literature [1–10]. For most of the bounds, Pan [11] has characterized the graphs which achieve the upper bounds of the largest Laplacian eigenvalues for unweighted graphs.

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Theorem 1 (*Rayleigh–Ritz* [12]). Let $A \in M_n$ be Hermitian, and let the eigenvalues of A be ordered such that $\lambda_n \leq \lambda_{n-1} \leq \cdots \leq \lambda_1$. Then,

$$\lambda_n x^T x \le x^T A x \le \lambda_1 x^T x$$

$$\lambda_{\max} = \lambda_1 = \max_{x \ne 0} \frac{x^T A x}{x^T x} = \max_{x^T x = 1} x^T A x$$

$$\lambda_{\min} = \lambda_n = \min_{x \ne 0} \frac{x^T A x}{x^T x} = \min_{x^T x = 1} x^T A x$$

for all $x \in \mathbb{C}^n$.

Proposition 1 ([13]). Let $A \in M_n$ have eigenvalues $\{\lambda_i\}$. Even if A is not Hermitian, one has the bounds

$$\min_{x \neq 0} \left| \frac{x^T A x}{x^T x} \right| \le |\lambda_i| \le \max_{x \neq 0} \left| \frac{x^T A x}{x^T x} \right|$$
(1.1)

for i = 1, 2, ..., n.

Corollary 1 ([13]). Let $A \in M_n$ have eigenvalues $\{\lambda_i\}$. Even if A is not Hermitian, one has the bounds

$$\min_{x \neq 0, \ y \neq 0} \left| \frac{x^T A y}{x^T y} \right| \le |\lambda_i| \le \max_{x \neq 0, \ y \neq 0} \left| \frac{x^T A y}{x^T y} \right|$$
(1.2)

for any $\bar{x} \in \mathbb{R}^n (\bar{x} \neq \bar{0}), \bar{y} \in \mathbb{R}^n (\bar{y} \neq \bar{0})$ and for i = 1, 2, ..., n.

Lemma 1 (Horn and Johnson [12]). Let B be a Hermitian $n \times n$ matrix with eigenvalues $\lambda_1 \ge \lambda_2 \ge \cdots \ge \lambda_n$, then for any $\bar{x} \in R^n(\bar{x} \neq \bar{0}), \bar{y} \in R^n(\bar{y} \neq \bar{0})$,

$$\left|\bar{x}^{T}B\bar{y}\right| \leq \lambda_{1}\sqrt{\bar{x}^{T}\bar{x}}\sqrt{\bar{y}^{T}\bar{y}}.$$
(1.3)

Equality holds if and only if \bar{x} is an eigenvector of B corresponding to λ_1 and $\bar{y} = \alpha \bar{x}$ for some $\alpha \in R$.

Some upper bounds on the largest Laplacian eigenvalue for weighted graphs, where the edge weights are positive definite matrices, are known as below. Then, we also give an upper bound on the largest Laplacian eigenvalue for weighted graphs in Section 2 and compare our bound with other bounds.

Theorem 2 (Das and Bapat [14]). Let G be a simple connected weighted graph. Then

$$\lambda_1 \le \max_{i \sim j} \left\{ \lambda_1 \left(\sum_{k:k \sim i} w_{ik} \right) + \sum_{k:k \sim j} \lambda_1(w_{jk}) \right\}$$
(1.4)

where w_{ij} is the positive definite weight matrix of order p of the edge ij. Moreover equality holds in (1.4) if and only if

(i) G is a weight-semiregular bipartite graph;

(ii) w_{ij} have a common eigenvector corresponding to the largest eigenvalue $\lambda_1(w_{ij})$ for all *i*, *j*.

Theorem 3 (Das [15]). Let G be a simple connected weighted graph. Then

$$\lambda_{1} \leq \max_{i \sim j} \left\{ \sqrt{\sum_{k:k \sim i} \lambda_{1}(w_{ik}) \left(\sum_{r:r \sim i} \lambda_{1}(w_{ir}) + \sum_{s:s \sim k} \lambda_{1}(w_{ks}) \right) + \sum_{k:k \sim j} \lambda_{1}(w_{jk}) \left(\sum_{r:r \sim j} \lambda_{1}(w_{jr}) + \sum_{s:s \sim k} \lambda_{1}(w_{ks}) \right) \right\}$$
(1.5)

where w_{ij} is the positive definite weight matrix of order p of the edge ij. Moreover equality holds in (1.5) if and only if

(i) G is a bipartite semiregular graph; and

. .

(ii) w_{ij} have a common eigenvector corresponding to the largest eigenvalue $\lambda_1(w_{ij})$ for all i, j.

Theorem 4 (Das [15]). Let G be a simple connected weighted graph. Then

$$\lambda_1 \le \max_{i \sim j} \left\{ \frac{\lambda_1(w_i) + \lambda_1(w_j) + \sqrt{(\lambda_1(w_i) - \lambda_1(w_j))^2 + 4\bar{\gamma}_i \bar{\gamma}_j}}{2} \right\}$$
(1.6)

where $\bar{\gamma}_i = \frac{\sum_{k:k \sim i} \lambda_1(w_{ik})\lambda_1(w_k)}{\lambda_1(w_i)}$ and w_{ij} is the positive definite weight matrix of order p of the edge ij. Moreover equality holds in (1.6) if and only if

(i) *G* is a weighted-regular graph or *G* is a weight-semiregular bipartite graph;

(ii) w_{ii} have a common eigenvector corresponding to the largest eigenvalue $\lambda_1(w_{ii})$ for all i, j.

2. An upper bounds on the largest Laplacian eigenvalue of weighted graphs

Theorem 5. Let G be a simple connected weighted graph. Then

$$\lambda_{1} \leq \max_{i} \left\{ \sqrt{\lambda_{1}^{2}(w_{i}) + \sum_{k:k\sim i} \lambda_{1}^{2}(w_{ik}) + \sum_{k:k\sim i} \lambda_{1}(w_{i}w_{ik} + w_{ik}w_{k}) + \sum_{1 \leq i,t \leq n} \sum_{s \in N_{i} \cap N_{t}} \lambda_{1}(w_{is}w_{st})} \right\}$$
(2.1)

`

where w_{ik} is the positive definite weight matrix of order p of the edge ik and $N_i \cap N_k$ is the set of common neighbours of i and k. Moreover equality holds in (2.1) if and only if

- (i) *G* is a weighted-regular graph or *G* is a weight-semiregular bipartite graph;
- (ii) w_{ik} have a common eigenvector corresponding to the largest eigenvalue $\lambda_1(w_{ik})$ for all *i*, *k*.

Proof. Let $\bar{X} = (\bar{x}_1^T, \bar{x}_2^T, \dots, \bar{x}_n^T)^T$ be an eigenvector corresponding to the largest eigenvalue λ_1 of L(G). We assume that \bar{x}_i is the vector component of \bar{X} such that

$$\bar{x}_i^T \bar{x}_i = \max_{k \in V} \left\{ \bar{x}_k^T \bar{x}_k \right\}.$$

$$(2.2)$$

Since \bar{X} is nonzero, so is \bar{x}_i .

The (i, j)-th element of L(G) is

$$\begin{cases} w_i; & \text{if } i = j \\ -w_{i,j}; & \text{if } i \sim j \\ 0; & \text{otherwise.} \end{cases}$$

Now we consider the matrix $L^2(G)$. The (i, j)-th element of $L^2(G)$ is

$$\begin{cases} w_i^2 + \sum_{k \in N_i} w_{ik}^2; & \text{if } i = j \\ -w_i w_{ij} - w_{ji} w_j + \sum_{k \in N_i \cap N_j} w_{ik} w_{kj}; & \text{otherwise.} \end{cases}$$

We have

$$L^2(G)\bar{X} = \lambda_1^2 \bar{X}.$$
(2.3)

From the i-th equation of (2.3), we have

$$\lambda_{1}^{2}\bar{x}_{i} = w_{i}^{2}\bar{x}_{i} + \sum_{k:k\sim i} w_{ik}^{2}\bar{x}_{i} + \sum_{k:k\sim i} -(w_{i}w_{ik} + w_{ik}w_{k})\bar{x}_{k} + \sum_{1\leq i,t\leq n} \left(\sum_{s\in N_{i}\cap N_{t}} w_{is}w_{st}\bar{x}_{t}\right)$$

i.e.

$$\lambda_{1}^{2} \bar{x}_{i}^{T} \bar{x}_{i} = \bar{x}_{i}^{T} w_{i}^{2} \bar{x}_{i} + \sum_{k:k\sim i} \bar{x}_{i}^{T} w_{ik}^{2} \bar{x}_{i} + \sum_{k:k\sim i} -\bar{x}_{i}^{T} \left((w_{i}w_{ik} + w_{ki}w_{k}) \right) \bar{x}_{k} + \sum_{1 \le i,t \le n} \left(\sum_{s \in N_{i} \cap N_{t}} \bar{x}_{i}^{T} w_{is} w_{st} \bar{x}_{t} \right).$$

$$(2.4)$$

Taking the modulus on both sides of (2.4), we get

$$\left|\lambda_{1}^{2}\left|\bar{x}_{i}^{T}\bar{x}_{i}\leq\left|\bar{x}_{i}^{T}w_{i}^{2}\bar{x}_{i}\right|+\sum_{k:k\sim i}\left|\bar{x}_{i}^{T}w_{ik}^{2}\bar{x}_{i}\right|+\sum_{k\sim i}\left|\bar{x}_{i}^{T}(w_{i}w_{ik}+w_{ki}w_{k})\bar{x}_{k}\right|+\sum_{1\leq i,t\leq n}\left(\sum_{s\in N_{i}\cap N_{t}}\left|\bar{x}_{i}^{T}w_{is}w_{st}\bar{x}_{t}\right|\right).$$
(2.5)

Since $w_{i,k}$ is the positive definite matrix for every $i, k, w_{i,k}^2$ matrices are also positive definite. So, we have

$$\leq \lambda_{1}(w_{i}^{2})\bar{\mathbf{x}}_{i}^{T}\bar{\mathbf{x}}_{i} + \sum_{k:k\sim i}\lambda_{1}(w_{ik}^{2})\bar{\mathbf{x}}_{i}^{T}\bar{\mathbf{x}}_{i} + \sum_{k\sim i}\left|\bar{\mathbf{x}}_{i}^{T}(w_{i}w_{ik} + w_{ik}w_{k})\bar{\mathbf{x}}_{k}\right| + \sum_{1\leq i,t\leq n}\left(\sum_{s\in N_{i}\cap N_{t}}\left|\bar{\mathbf{x}}_{i}^{T}w_{is}w_{st}\bar{\mathbf{x}}_{t}\right|\right)$$
(2.6)

from (1.3).

Now let examine whether $(w_i w_{ik} + w_{ki} w_k)$ for $k \sim i$ and $w_{is} w_{st}$ for $s \in N_i \cap N_t$ are Hermitian in the inequality of (2.6). Case 1: $(w_i w_{ik} + w_{ki} w_k)$ and $w_{is} w_{st}$ are Hermitian matrices. Then using inequality in (1.3), we get (2.6) as

$$\leq \lambda_{1}(w_{i}^{2})\bar{\mathbf{x}}_{i}^{T}\bar{\mathbf{x}}_{i} + \sum_{k:k\sim i}\lambda_{1}(w_{ik}^{2})\bar{\mathbf{x}}_{i}^{T}\bar{\mathbf{x}}_{i} + \sum_{k\sim i}\lambda_{1}(w_{i}w_{ik} + w_{ki}w_{k})\sqrt{\bar{\mathbf{x}}_{i}^{T}\bar{\mathbf{x}}_{i}}\sqrt{\bar{\mathbf{x}}_{k}^{T}\bar{\mathbf{x}}_{k}} + \sum_{1\leq i,t\leq n}\left(\sum_{s\in N_{i}\cap N_{t}}\lambda_{1}(w_{is}w_{st})\sqrt{\bar{\mathbf{x}}_{i}^{T}\bar{\mathbf{x}}_{i}}\sqrt{\bar{\mathbf{x}}_{t}^{T}\bar{\mathbf{x}}_{i}}\right).$$

$$(2.7)$$

Case 2: $(w_i w_{ik} + w_{ki} w_k)$ is Hermitian for $k \sim i$ and $w_{is} w_{st}$ is not a Hermitian matrix for $s \in N_i \cap N_t$, $1 \le i$, $t \le n$. Since $(w_i w_{ik} + w_{ki} w_k)$ is Hermitian, from (1.3) we have

$$\sum_{k \sim i} \left| \bar{\mathbf{x}}_{i}^{T}(w_{i}w_{ik} + w_{ki}w_{k})\bar{\mathbf{x}}_{k} \right| \leq \lambda_{1}((w_{i}w_{ik} + w_{ki}w_{k}))\sqrt{\bar{\mathbf{x}}_{i}^{T}\bar{\mathbf{x}}_{i}}\sqrt{\bar{\mathbf{x}}_{k}^{T}\bar{\mathbf{x}}_{k}}.$$
(2.8)

Now, let $w_{is}w_{st}$ not be a Hermitian matrix for $s \in N_i \cap N_t$, $1 \le i, t \le n$. Let us take the ratio of

$$(2.9)$$

for $1 \le k, t \le n$. If $N_k \cap N_t = \emptyset$, this ratio is zero. So let us consider $N_k \cap N_t \ne \emptyset$. Then we get

$$\left|\frac{\bar{x}_k^T w_{ks} w_{st} \bar{x}_t}{\bar{x}_k^T \bar{x}_t}\right| = \frac{\left|\bar{x}_k^T w_{ks} w_{st} \bar{x}_t\right|}{\left|\bar{x}_k^T \bar{x}_t\right|}$$

and using the Cauchy Schwarz inequality we have

$$\geq \frac{\left|\bar{x}_{k}^{T} w_{ks} w_{st} \bar{x}_{t}\right|}{\sqrt{\bar{x}_{k}^{T} \bar{x}_{k}} \sqrt{\bar{x}_{t}^{T} \bar{x}_{t}}}.$$

From (2.2), we get

$$\left|\frac{\bar{x}_k^T w_{ks} w_{st} \bar{x}_t}{\bar{x}_k^T \bar{x}_t}\right| \ge \frac{\left|\bar{x}_k^T w_{ks} w_{st} \bar{x}_t\right|}{\sqrt{\bar{x}_i^T \bar{x}_i} \sqrt{\bar{x}_t^T \bar{x}_t}}.$$
(2.10)

Since (2.10) implies for each \bar{x}_k and \bar{x}_t

$$\min_{\bar{x}_k \neq 0, \bar{x}_t \neq 0} \left\{ \left| \frac{\bar{x}_k^T w_{ks} w_{st} \bar{x}_t}{\bar{x}_k^T \bar{x}_t} \right| \right\} = \frac{\left| \bar{x}_i^T w_{ks} w_{st} \bar{x}_t \right|}{\sqrt{\bar{x}_i^T \bar{x}_i} \sqrt{\bar{x}_i^T \bar{x}_t}}$$

from inequality of (1.2) and since λ_1 ($w_{is}w_{st}$) is the largest eigenvalue of $w_{is}w_{st}$ matrix for $s \in N_i \cap N_t$, $1 \le i, t \le n$ we have

$$\frac{\left|\bar{x}_{i}^{T}w_{is}w_{st}\bar{x}_{t}\right|}{\sqrt{\bar{x}_{i}^{T}\bar{x}_{i}}\sqrt{\bar{x}_{t}^{T}\bar{x}_{t}}} \leq \left|\lambda_{i}\right|\left(w_{is}w_{st}\right) \leq \lambda_{1}\left(w_{is}w_{st}\right),$$
(2.11)

i.e.

$$\sum_{1 \le i,t \le n} \sum_{s \in N_i \cap N_t} \left| \bar{x}_i^T w_{is} w_{st} \bar{x}_t \right| \le \lambda_1 \left(w_{is} w_{st} \right) \sqrt{\bar{x}_i^T \bar{x}_i} \sqrt{\bar{x}_t^T \bar{x}_t}.$$
(2.12)

If we arrange the expressions (2.8) and (2.12) in the inequality of (2.6), we can again get the inequality in (2.7). Case 3: $(w_i w_{ik} + w_{ki} w_k)$ is not Hermitian for $k \sim i$ and $w_{is} w_{st}$ is a Hermitian matrix for $s \in N_i \cap N_t$, $1 \le i$, $t \le n$. Since the matrix of $w_{is} w_{st}$ is Hermitian, we get

$$\sum_{1 \le i,t \le n} \left(\sum_{s \in N_i \cap N_t} \left| \bar{x}_i^T w_{is} w_{st} \bar{x}_t \right| \right) \le \sum_{1 \le i,t \le n} \left(\sum_{s \in N_i \cap N_t} \lambda_1 \left(w_{is} w_{st} \right) \sqrt{\bar{x}_i^T \bar{x}_i} \sqrt{\bar{x}_t^T \bar{x}_t} \right).$$

$$(2.13)$$

On the other hand, let $(w_i w_{ik} + w_{ki} w_k)$ not be a Hermitian matrix for $k \sim i$. By a similar argument to Case 2 we have

$$\frac{\left|\bar{x}_{i}^{T}(w_{i}w_{ik}+w_{ki}w_{k})\bar{x}_{t}\right|}{\sqrt{\bar{x}_{i}^{T}\bar{x}_{i}}\sqrt{\bar{x}_{k}^{T}\bar{x}_{k}}} \leq |\lambda_{i}|\left(w_{i}w_{ik}+w_{ki}w_{k}\right) \leq \lambda_{1}\left(w_{i}w_{ik}+w_{ki}w_{k}\right),$$
(2.14)

i.e.

$$\sum_{k \sim i} \left| \bar{x}_{i}^{T}(w_{i}w_{ik} + w_{ki}w_{k})\bar{x}_{k} \right| \leq \sum_{k \sim i} \lambda_{1} \left(w_{i}w_{ik} + w_{ki}w_{k} \right) \sqrt{\bar{x}_{i}^{T}\bar{x}_{i}} \sqrt{\bar{x}_{k}^{T}\bar{x}_{k}}.$$
(2.15)

If we arrange the expressions (2.15) and (2.13) in the inequality of (2.6), we can again get the inequality in (2.7). Case 4: The matrices of $(w_iw_{ik} + w_{ki}w_k)$ for $k \sim i$ and $w_{is}w_{st}$ for $s \in N_i \cap N_t$, $1 \le i$, $t \le n$ are not Hermitian matrices. By applying the same methods as Cases 2 and 3, we have also (2.7). Therefore, we see that

$$\lambda_{1}^{2} \bar{x}_{i}^{T} \bar{x}_{i} \leq \lambda_{1}(w_{i}^{2}) \bar{x}_{i}^{T} \bar{x}_{i} + \sum_{k:k\sim i} \lambda_{1}(w_{ik}^{2}) \bar{x}_{i}^{T} \bar{x}_{i} + \sum_{k\sim i} \lambda_{1}(w_{ik}w_{ik} + w_{ki}w_{k}) \sqrt{\bar{x}_{i}^{T} \bar{x}_{i}} \sqrt{\bar{x}_{k}^{T} \bar{x}_{k}} + \sum_{1 \leq i,t \leq n} \left(\sum_{s \in N_{i} \cap N_{t}} \lambda_{1}(w_{is}w_{st}) \sqrt{\bar{x}_{i}^{T} \bar{x}_{i}} \sqrt{\bar{x}_{t}^{T} \bar{x}_{t}} \right)$$

$$(2.16)$$

in all situations. If we use (2.2), we have

$$\leq \lambda_{1}(w_{i}^{2})\bar{x}_{i}^{T}\bar{x}_{i} + \sum_{k:k\sim i}\lambda_{1}(w_{ik}^{2})\bar{x}_{i}^{T}\bar{x}_{i} + \sum_{k\sim i}\lambda_{1}(w_{i}w_{ik} + w_{ki}w_{k})\bar{x}_{i}^{T}\bar{x}_{i} + \sum_{1\leq i,t\leq n}\sum_{s\in N_{i}\cap N_{t}}\lambda_{1}(w_{is}w_{st})\bar{x}_{i}^{T}\bar{x}_{i}.$$
(2.17)

Thus we obtain

$$\lambda_{1} \leq \sqrt{\lambda_{1}(w_{i}^{2}) + \sum_{k:k \sim i} \lambda_{1}(w_{i,k}^{2}) + \sum_{k \sim i} \lambda_{1}(w_{i}w_{ik} + w_{ki}w_{k}) + \sum_{1 \leq i,t \leq n} \sum_{s \in N_{i} \cap N_{t}} \lambda_{1}(w_{i,s}w_{s,t})}$$

i.e.

$$\lambda_1 \le \max_{i \in V} \left\{ \sqrt{\left(\lambda_1(w_i^2) + \sum_{k:k \sim i} \lambda_1(w_{ik}^2) + \sum_{k \sim i} \lambda_1(w_i w_{ik} + w_{ki} w_k) + \sum_{1 \le i, t \le n} \sum_{s \in N_i \cap N_t} \lambda_1(w_{is} w_{st}) \right) \right\}.$$

$$(2.18)$$

Now suppose that equality in (2.1) holds. Then all the equalities in the above argument must be equalities. From equality in (2.17) we have

$$\bar{\mathbf{x}}_i^T \bar{\mathbf{x}}_i = \bar{\mathbf{x}}_k^T \bar{\mathbf{x}}_k \tag{2.19}$$

for all $k, k \sim i$ and for all $k, k \sim p, p \sim i$. From this we say $\bar{x}_k \neq \bar{0}$.

From equality in (2.16) and using Lemma 1 we get that \bar{x}_i is eigenvector of $w_{i,k}$, $(w_i w_{ik} + w_{ki} w_k)$, $w_{is} w_{sk}$ such that $s \in N_i \cap N_k$ for the largest eigenvalues $\lambda_1(w_{ik})$, $\lambda_1(w_i w_{ik} + w_{ki} w_k)$, $\lambda_1(w_{is} w_{sk})$ respectively and for any k

$$\bar{x}_k = b_{ik}\bar{x}_i \tag{2.20}$$

for some b_{ik} . Similarly, from equality in (2.16) and using Lemma 1 we also get that \bar{x}_i is an eigenvector of $w_{is}w_{st}$ such that $s \in N_i \cap N_t$ for the largest eigenvalue $\lambda_1(w_{is}w_{st})$ for any $1 \le i, t \le n$

$$\bar{\mathbf{x}}_t = c_{it}\bar{\mathbf{x}}_i \tag{2.21}$$

for some c_{it} .

From (2.19) we get

$$(b_{ik}^2 - 1) \, \bar{x}_i^T \bar{x}_i = 0 \, (c_{it}^2 - 1) \, \bar{x}_i^T \bar{x}_i = 0$$

i.e.

$$b_{ik} = \pm 1, \qquad c_{it} = \pm 1 \quad \text{as } \bar{x}_i^T \bar{x}_i > 0.$$
 (2.22)

Now let's take any vertex *i*.

Since w_{ik} is a positive definite matrix, w_{ik}^2 and w_i^2 are also positive matrices. Thus, we get

$$\bar{x}_{i}^{T}w_{i}^{2}\bar{x}_{i} > 0,$$

 $\bar{x}_{i}^{T}w_{ik}^{2}\bar{x}_{i} > 0.$ (2.23)

From equality in (2.16) we get

$$-\sum_{k\sim i} b_{ik} \bar{x}_{i}^{T} \left(w_{i} w_{ik} + w_{ki} w_{k} \right) \bar{x}_{i} = \sum_{k\sim i} |b_{ik}| \left| \bar{x}_{i}^{T} \left(w_{i} w_{ik} + w_{ki} w_{k} \right) \bar{x}_{i} \right|$$
(2.24)

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and

$$\sum_{1 \le i,t \le n} \sum_{s \in N_i \cap N_t} c_{it} \bar{x}_i^T w_{is} w_{st} \bar{x}_i = \sum_{1 \le i,t \le n} \sum_{s \in N_i \cap N_t} |c_{it}| \left| \bar{x}_i^T w_{is} w_{st} \bar{x}_i \right|.$$

$$(2.25)$$

Since $b_{ik} = \pm 1$, therefore from (2.24), we get $b_{ik} = -1$ for all $k, k \sim i$. Hence,

$$\bar{x}_k = -\bar{x}_i$$

for all $k, k \sim i$.

Since $c_{it} = \pm 1$, therefore from (2.25) we get $c_{it} = 1$ for all $1 \le i, t \le n$. Hence,

$$\bar{x}_t = \bar{x}_i$$

for all $1 \le i, t \le n$.

Let $U = \{k : \bar{x}_k = -\bar{x}_i\}$ for all $k, k \sim i$ and $W = \{k : \bar{x}_k = \bar{x}_i\}$ such that $k \in N_i \cap N_t$ for all $1 \leq i, t \leq n$. Moreover, from equality in (2.17), \bar{x}_i is a common eigenvector of $w_{i,k}$, corresponding to the largest eigenvalue $\lambda_1(w_{ik})$ for all i, k. Since G is connected $V = U \cup W$ and the subgraphs induced by U and W respectively are empty graphs. Hence G is bipartite. Now we have

$$L(G)\bar{x}_i = \lambda_1 \bar{x}_i, \tag{2.26}$$

i.e.

$$w_i \bar{x}_i - \sum_{k:k\sim i} w_{ik} \bar{x}_k = \lambda_1 \bar{x}_i.$$
(2.27)

For $i, p \in U$

$$\lambda_1 \bar{x}_i = w_i \bar{x}_i + \sum_{k:k\sim i} w_{ik} \bar{x}_i \tag{2.28}$$

and

$$\lambda_1 \bar{x}_i = w_p \bar{x}_i + \sum_{k:k\sim p} w_{ip} \bar{x}_i.$$
(2.29)

So, we get

$$\left(\lambda_1(w_i) - \lambda_1(w_p)\right) x_i = 0 \tag{2.30}$$

from (2.28) and (2.29) as \bar{x}_i is an eigenvector of w_i corresponding to the largest eigenvalue $\lambda_1(w_i)$ for all i. Since $\bar{x}_i \neq 0$, therefore $\lambda_1(w_i)$ is constant for all $i \in U$. Similarly we can also show that $\lambda_1(w_i)$ is constant for all $i \in W$. Hence G is a bipartite semiregular graph.

Conversely, suppose that conditions (i)–(ii) of the theorem hold for the graph G. We must prove

$$\lambda_{1} = \max_{i} \left\{ \sqrt{\lambda_{1}^{2}(w_{i}) + \sum_{k:k\sim i} \lambda_{1}^{2}(w_{ik}) + \sum_{k:k\sim i} \lambda_{1}(w_{i}w_{ik} + w_{ki}w_{k}) + \sum_{1 \le i,t \le n} \sum_{s \in N_{i} \cap N_{t}} \lambda_{1}(w_{is}w_{st})} \right\}.$$

Let *U*, *W* be partite sets of *G*. Also let $\lambda_1(w_i) = \alpha$ for $i \in U$ and $\lambda_1(w_i) = \beta$ for $i \in W$.

Since *G* is a bipartite graph, therefore *U*, *W* are partite sets of *G*. $N_i \cap N_t$ is empty for all $1 \le i, t \le n$. To prove, let $N_i \cap N_t \ne \emptyset$. Thus, there is a vertex *s* such that $s \sim i, s \sim t$. On the other hand, let $i \in U, t \in W$.

$$s \sim i \Rightarrow s \in W \tag{2.31}$$

$$s \sim t \Rightarrow s \in U. \tag{2.32}$$

This is contradiction according to (2.30) and (2.31). Hence, we found that $N_i \cap N_t = \emptyset$. The following equation can be easily verified:

$$(2\alpha^{2} + 2\alpha\beta)\begin{pmatrix} \bar{x}\\ \bar{x}\\ \vdots\\ \bar{x}\\ -\bar{x}\\ -\bar{x}\\ \vdots\\ -\bar{x} \end{pmatrix} = A\begin{pmatrix} \bar{x}\\ \bar{x}\\ \vdots\\ \bar{x}\\ -\bar{x}\\ -\bar{x}\\ \vdots\\ -\bar{x} \end{pmatrix}$$

where

$$A = \begin{pmatrix} w_1^2 + \sum_{k \in N_1} w_{1,n}^2 & -(w_1 w_{1,2} + w_{1,2} w_2) + \sum_{k \in N_1 \cap N_2} w_{1k} w_{k,2} \cdots & -(w_1 w_{1,n} + w_{1,n} w_n) + \sum_{k \in N_1 \cap N_n} w_{1,k} w_{k,n} \\ -(w_2 w_{1,2} + w_{1,2} w_1) + \sum_{k \in N_1 \cap N_2} w_{1,k} w_{k,2} & w_2^2 + \sum_{k \in N_2} w_{1,2}^2 \cdots & -(w_2 w_{1,n} + w_{1,n} w_n) + \sum_{k \in N_2 \cap N_n} w_{2,k} w_{k,n} \\ \vdots & \vdots & \vdots & \vdots \\ -(w_n w_{1,n} + w_{1,n} w_1) + \sum_{k \in N_1 \cap N_n} w_{1,k} w_{k,n} & -(w_2 w_{1,n} + w_{1,n} w_n) + \sum_{k \in N_2 \cap N_n} w_{2,k} w_{k,n} \cdots & w_n^2 + \sum_{k \in N_n} w_{k,n}^2 \end{pmatrix}.$$

Therefore $2\alpha^2 + 2\alpha\beta$ is an eigenvalue of $L^2(G)$. So

$$2\alpha^2 + 2\alpha\beta \le \lambda_1^2. \tag{2.33}$$

On the other hand, we have

$$\lambda_{1}^{2}(w_{i}) + \sum_{k:k\sim i} \lambda_{1}^{2}(w_{ik}) + \sum_{k:k\sim i} \lambda_{1}(w_{i}w_{ik} + w_{ik}w_{k}) + \sum_{1 \le i,t \le n} \sum_{s \in N_{i} \cap N_{t}} \lambda_{1}(w_{is})\lambda_{1}(w_{st}) = 2\alpha^{2} + 2\alpha\beta$$
(2.34)

for all $i \in V$. We get

$$\lambda_{1}^{2} \leq \max_{i \in V} \left\{ \left(\lambda_{1}(w_{i}^{2}) + \sum_{k:k \sim i} \lambda_{1}(w_{ik}^{2}) + \sum_{k \sim i} \lambda_{1}((w_{i}w_{ik} + w_{ik}w_{k})) + \sum_{1 \leq i, t \leq n} \sum_{s \in N_{i} \cap N_{t}} \lambda_{1}(w_{is}w_{sk}) \right) \right\} = 2\alpha^{2} + 2\alpha\beta$$

from inequality in (2.18). Hence the theorem is proved by (2.33). $\hfill\square$

Corollary 2. Let G be a simple connected weighted graph where each edge weight $w_{i,j}$ is a positive number. Then

$$\lambda_{1} \leq \max_{i} \left\{ \sqrt{w_{i}^{2} + w_{i} + \sum_{j} \left\{ (w_{i}w_{i,j} + w_{i,j}w_{j}) : i \sim j \right\} + \sum_{1 \leq i, t \leq n} \sum_{s} \left\{ w_{is}w_{sj} : s \in N_{i} \cap N_{t} \right\}} \right\}.$$
(2.35)

`

Moreover equality holds in (2.35) if and only if G is a bipartite semiregular graph.

Proof. We have $\lambda_1(w_i) = w_i$ and $\lambda_1(w_{ij}) = w_{ij}$ for all *i*, *j*. From Theorem 5 we get the required result. \Box

Corollary 3. Let G be a simple connected unweighted graph. Then

$$\lambda_{1} \leq \max_{i} \left\{ \sqrt{d_{i}^{2} + d_{i} + \sum_{j} \left\{ d_{i} + d_{j} + \left| N_{i} \cap N_{j} \right| : i \sim j \right\} + \sum_{j} \left\{ \left| N_{i} \cap N_{j} \right| : i \sim j \right\}} \right\}$$

where d_i is the degree of vertex i and $|N_i \cap N_i|$ is the number common neighbors of i and j.

Proof. For an unweighted graph, $w_{i,j} = 1$ for $i \sim j$. Therefore $w_i = d_i$. Using Corollary 2 we get the required results. \Box

Example 1. Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be a weighted graph where $V_1 = \{1, 2, 3, 4\}, E_1 = \{\{1, 4\}, \{2, 3\}, \{3, 4\}\}$ and each weight is a positive definite matrix of three order. Let $V_2 = \{1, 2, 3, 4, 5, 6, 7\}, E_2 = \begin{cases} \{1, 4\}, \{2, 4\}, \{3, 4\}, \{3, 4\}, \{4, 5\}, \{5, 6\}, \{5, 7\} \end{cases}$ such that each weight is a positive definite matrix of order two. Assume that the Laplacian matrices of G_1 and G_2 are as follows:

$$L(G_1) = \begin{bmatrix} 3 & 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & -3 & -1 & 1 \\ 1 & 3 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & -3 & 1 \\ -1 & -1 & 5 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & -5 \\ 0 & 0 & 0 & 5 & 0 & 2 & -5 & 0 & -2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 5 & 2 & 0 & -5 & -2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 & 2 & 5 & -2 & -2 & -5 & 0 & 0 & 0 \\ 0 & 0 & 0 & -5 & 0 & -2 & 6 & 0 & 2 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -5 & -2 & 0 & 10 & 5 & 0 & -5 & -3 \\ 0 & 0 & 0 & -2 & -2 & -5 & 2 & 5 & 8 & 0 & -3 & -3 \\ -3 & -1 & 1 & 0 & 0 & 0 & -1 & 0 & 0 & 4 & 1 & -1 \\ -1 & -3 & 1 & 0 & 0 & 0 & 0 & -5 & -3 & 1 & 8 & 2 \\ 1 & 1 & -5 & 0 & 0 & 0 & 0 & -3 & -3 & -1 & 2 & 8 \end{bmatrix}$$

and

	г1	1	0	0	0	0	-1	-1	0	0	0	0	0	0 т	
$L(G_2) =$	1	2	0	0	0	0	-1	$^{-2}$	0	0	0	0	0	0	
	0	0	1	1	0	0	-1	-1	0	0	0	0	0	0	
	0	0	1	3	0	0	-1	-3	0	0	0	0	0	0	
	0	0	0	0	1	1	-1	-1	0	0	0	0	0	0	
	0	0	0	0	1	4	-1	-4	0	0	0	0	0	0	
	-1	$^{-1}$	-1	-1	-1	-1	4	4	-1	-1	0	0	0	0	
	-1	-2	-1	-3	-1	-4	4	14	-1	-5	0	0	0	0	•
	0	0	0	0	0	0	-1	-1	3	3	-1	-1	-1	-1	
	0	0	0	0	0	0	-1	-5	3	18	-1	-6	-1	7	
	0	0	0	0	0	0	0	0	-1	-1	1	1	0	0	
	0	0	0	0	0	0	0	0	-1	-6	1	6	0	0	
	0	0	0	0	0	0	0	0	-1	-1	0	0	1	1	
	Lο	0	0	0	0	0	0	0	-1	-7	0	0	1	7]	

The largest eigenvalues of $L(G_1)$ and $L(G_2)$ are $\lambda_1 = 22.25$, $\lambda_2 = 26.16$ rounded two decimal places and the above mentioned bounds give the following results:

Consequently, we see that the bound in (2.1) is better than the bounds in (1.4) and (1.5). But it is not better than the bound in (1.6) from the above table.

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