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THE GRONE-MERRIS CONJECTURE

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Abstract. In spectral graph theory, the Grone-Merris Conjecture asserts that the spectrum of the Laplacian matrix of a finite graph is majorized by the conjugate degree sequence of this graph. We give a complete proof for this conjecture.

The Laplacian of a simple graph G with n vertices is a positive semi-definite $n \times n$ matrix $L(G)$ that mimics the geometric Laplacian of a Riemannian manifold; see §1 for definitions, and [2, 14] for comprehensive bibliographies on the graph Laplacian. The spectrum sequence $\lambda(G)$ of $L(G)$ can be listed in non-increasing order as

$$\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_{n-1}(G) \geq \lambda_n(G) = 0.$$

For two non-increasing real sequences $\mathbf{x}$ and $\mathbf{y}$ of length n, we say that $\mathbf{x}$ is *majorized* by $\mathbf{y}$ (denoted $\mathbf{x} \preccurlyeq \mathbf{y}$) if

$$\sum_{i=1}^{k} x_i \leq \sum_{i=1}^{k} y_i \text{ for all } k \leq n, \text{ and } \sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i.$$

This notion was introduced because of the following fundamental theorem.

Theorem 1 (Schur-Horn Dominance Theorem [18, 11]). *There exists a Hermitian matrix H with diagonal entry sequence $\mathbf{x}$ and spectrum sequence $\mathbf{y}$ if and only if $\mathbf{x} \preccurlyeq \mathbf{y}$.*

In particular, if $\mathbf{d}(G) = (d_1, d_2, \ldots, d_n)^T$ is the non-increasing *degree sequence* of G, which coincides with the diagonal entry sequence of the Laplacian matrix $L(G)$, the Schur-Horn Dominance Theorem implies that $\mathbf{d}(G) \preccurlyeq \lambda(G)$. Grone [7] improves this majorization result: if G has at least one edge, then $(d_1 + 1, d_2, \ldots, d_{n-1}, d_n - 1)^T \preccurlyeq \lambda(G)$.

For a non-negative integral sequence $\mathbf{d}$, we define its *conjugate degree sequence* as the sequence $\mathbf{d}' = (d'_1, d'_2, \ldots, d'_n)^T$ where

$$d'_k := \#\{i : d_i \geq k\}.$$

Another important majorization relation is the following.

Theorem 2 (Gale-Ryser [6, 17]). *There exists a $(0,1)$-matrix A with row and column sum vectors $\mathbf{r}$ and $\mathbf{c}$ if and only if $\mathbf{r} \preccurlyeq \mathbf{c}'$.*

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Applying this to the adjacency matrix of G immediately gives that $\mathbf{d}(G) \preccurlyeq \mathbf{d}'(G)$.

In 1994, Grone and Merris [8, 9] raised the natural question whether the Laplacian spectrum sequence and the conjugate degree sequence are majorization comparable.

Grone-Merris Conjecture. For any graph G, the Laplacian spectrum is majorized by the conjugate degree sequence

$$\lambda(G) \preccurlyeq \mathbf{d}'(G).$$

In this paper, we give a complete proof to the Grone-Merris Conjecture. As a consequence, we have the double majorization $\mathbf{d}(G) \preccurlyeq \lambda(G) \preccurlyeq \mathbf{d}'(G)$.

See [3] for a partial result in this direction, as well as [19, 12, 13, 1] for proofs in the special cases. Also see [3] for a generalization to simplicial complexes, which is still open.

1. The Laplacian matrix and the majorization relation

Let $G = (V, E)$ be a simple finite graph with $n = |V|$ vertices. We write $i \sim j$ when the i-th vertex is adjacent to the j-th vertex, and we let d_i denote the degree of the i-th vertex.

The *Laplacian matrix* $L(G)$ of the graph G is the $n \times n$ matrix defined by

$$L(G)_{ij} = \begin{cases} d_i & \text{if } i = j; \\ -1 & \text{if } i \sim j; \\ 0 & \text{otherwise.} \end{cases}$$

We can also express the Laplacian as $L(G) = D - A$, where D is the diagonal matrix defined by the degree sequence, and A is the adjacency $(0,1)$-matrix of the graph.

It is well known that $L(G)$ is positive semi-definite, since it corresponds to the quadratic form

$$\mathbf{x}^T L(G)\mathbf{x} = \sum_{i\sim j} (x_i - x_j)^2 \text{ for } \mathbf{x} = (x_1, \dots, x_n)^T \in \mathbb{R}^n.$$

Let $\lambda = (\lambda_1, \lambda_2, \dots, \lambda_n)^T$ be the non-increasing *spectrum sequence* of the Laplacian matrix $L(G)$. The smallest eigenvalue is $\lambda_n = 0$, with eigenvector $\mathbf{1}_n = (1, 1, \dots, 1)^T$.

Given two vectors $\mathbf{x} = (x_1, \dots, x_n)^T$ and $\mathbf{y} = (y_1, \dots, y_n)^T$ in $\mathbb{R}^n$, rearrange their components in non-increasing order as

$$x_{[1]} \geq x_{[2]} \geq \cdots \geq x_{[n]}, \quad y_{[1]} \geq y_{[2]} \geq \cdots \geq y_{[n]}.$$

We say that $\mathbf{x}$ is *majorized* by $\mathbf{y}$, and write $\mathbf{x} \preccurlyeq \mathbf{y}$, if

$$\sum_{i=1}^{k} x_{[i]} \leq \sum_{i=1}^{k} y_{[i]} \text{ for all } 1 \leq k \leq n, \text{ and } \sum_{i=1}^{n} x_i = \sum_{i=1}^{n} y_i.$$

We will make use of the following majorization inequality.

Theorem 3 (Fan [4])**.** *If H_1 and H_2 are Hermitian matrices, then*

$$\lambda(H_1 + H_2) \preccurlyeq \lambda(H_1) + \lambda(H_1).$$

2. Split graphs

A graph is *split* (also called *semi-bipartite* in [12]) if its vertices can be partitioned into a clique V_1 and a co-clique V_2. This is equivalent to saying that the subgraph induced by V_1 is complete, and that the subgraph induced by V_2 is an independent set. See [5, 20, 15, 10] for many characterizations and properties of split graphs.

Given a split graph $G = (V, E)$, let $N = |V_1|$ be the size of the clique, and $M = |V_2|$ be the size of the co-clique. Let $\delta(G)$ be the maximum degree of vertices in V_2. Clearly $\delta(G) \leq N$, and the Laplacian matrix of the split graph G is of the form

$$L(G) = \begin{pmatrix} K_N + D_1 & -A \\ -A^T & D_2 \end{pmatrix},$$

where K_N is the Laplacian matrix of the complete graph on N vertices, where D_1 and D_2 are diagonal matrices with diagonal entries the vertex degrees of V_1, V_2, respectively, and where A is the adjacency matrix for edges between V_1 and V_2.

The Laplacian matrix is symmetric, and therefore Hermitian.

Theorem 4 (Courant-Fischer-Weyl [16])**.** *Let the $n \times n$ matrix H be Hermitian, with eigenvalues $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. Then*

$$\lambda_k = \max_{\dim(S)=k} \min_{0 \neq x \in S} \frac{\langle Hx, x\rangle}{\langle x, x\rangle} = \min_{\dim(S)=n-k+1} \max_{0 \neq x \in S} \frac{\langle Hx, x\rangle}{\langle x, x\rangle},$$

where the max *(resp.* min*) is taken over all k-dimensional (resp. $(n-k+1)$-dimensional) subspaces of $\mathbb{R}^n$.*

We first investigate the Laplacian spectrum of a split graph.

Proposition 5. *If G is a split graph of clique size N, then*

$$\lambda_{N-1}(G) \geq N \geq \delta(G) \geq \lambda_{N+1}(G).$$

Moreover, if $\lambda_N(G) \geq N$, then

$$\sum_{i=1}^{N} d_i' = N^2 + \operatorname{Tr}(D_1).$$

Proof. To prove the inequalities involving $\lambda_{N-1}(G)$ and $\lambda_{N+1}(G)$ by the Courant-Fischer-Weyl Min-Max Principle, it suffices to find an $(N-1)$-dimensional (resp. M-dimensional) subspace for which the action of $L(G)$ has a desirable lower (resp. upper) bound. There are natural candidates.

Let $P \subset \mathbb{R}^{M+N}$ be the $(N-1)$-dimensional subspace consisting of all vectors of the form $\begin{pmatrix} u \\ \mathbf{0}_M \end{pmatrix}$ with $u \in \mathbb{R}^N$ and $u \perp \mathbf{1}_N$. Then for any unit vector $u \in \mathbb{R}^n$,

$$\left\langle L(G)\begin{pmatrix} u \\ \mathbf{0}_M \end{pmatrix}, \begin{pmatrix} u \\ \mathbf{0}_M \end{pmatrix}\right\rangle = \langle (K_N + D_1)u, u\rangle = N + \langle D_1 u, u\rangle \geq N.$$

Similarly, consider the M-dimensional subspace $Q \subset \mathbb{R}^{M+N}$ consisting of all vectors of the form $\begin{pmatrix} \mathbf{0}_N \\ u \end{pmatrix}$ with $u \in \mathbb{R}^M$. Then for any unit vector u,

$$\left\langle L(G)\begin{pmatrix} \mathbf{0}_N \\ u \end{pmatrix}, \begin{pmatrix} \mathbf{0}_N \\ u \end{pmatrix}\right\rangle = \langle D_2 u, u\rangle \leq \delta(G).$$

This proves the part of our first statement that $\lambda_{N-1}(G) \geq N \geq \delta(G) \geq \lambda_{N+1}(G)$.

When $\lambda_N(G) \geq N$, we assert that the degree of any vertex in the clique V_1 is at least N. For this, suppose that our assertion is false, namely that there exists a vertex $v_0 \in V_1$ with degree less than N. Then this vertex v_0 is adjacent to none of the vertices of the co-clique V_2. Consequently G can be regarded as a split graph with new clique $V_1 \setminus \{v_0\}$ and new co-clique $V_2 \cup \{v_0\}$. The size of the new clique is $\widetilde{N} = N - 1$. Applying the first part of the proposition, we obtain that

$$\lambda_N(G) = \lambda_{\widetilde{N}+1}(G) \leq \widetilde{N} = N - 1,$$

which is a contradiction.

For a conjugating pair of non-negative integral sequences, the partial sum of one sequence can be computed in a different way as

$$\sum_{i=1}^{N} d'_i = \sum_{i=1}^{N} \sum_{j=1}^{M+N} \chi(d_j \geq i) = \sum_{j=1}^{M+N} \min(d_j, N),$$

where χ is the characteristic function. The second part of the proposition now follows from the observation that

$$\sum_{j=1}^{M+N} \min(d_j, N) = \sum_{j \in V_1} N + \sum_{j \in V_2} d_j = N^2 + \mathrm{Tr}(D_2) = N^2 + \mathrm{Tr}(D_1). \qquad \square$$

The next lemma will play an essential role in our proof of the Grone-Merris Conjecture. Its proof is presented in the next section.

Lemma 6. *Assume that G is a split graph of clique size N. If either $\lambda_N(G) > N$ or $\lambda_N(G) = N > \delta(G)$, then the N-th inequality of the Grone-Merris Conjecture holds, namely*

$$\sum_{i=1}^{N} \lambda_i \leq \sum_{i=1}^{N} d'_i.$$

3. The homotopy method

This section is devoted to proving Lemma 6. We adopt a homotopy method, following an idea of Katz [12] in his proof of the Grone-Merris Conjecture for 1-regular semi-bipartite graph.

Let $\alpha \in [0, 1]$. Define an $(M + N) \times (M + N)$ matrix L_α as

$$L_\alpha = (1 - \alpha) \begin{pmatrix} K_N + M & -J_{N \times M} \\ -J_{M \times N} & N \end{pmatrix} + \alpha \begin{pmatrix} K_N + D_1 & -A \\ -A^T & D_2 \end{pmatrix},$$

where $J_{M \times N}$ denotes the $M \times N$ matrix whose entries are all equal to 1.

Note that $L_1 = L(G)$ is the matrix we are interested in, and that L_0 is the Laplacian of a complete split graph. The spectrum of L_0 is well understood:

Lemma 7. *The Laplacian spectrum of the complete split graph of clique size N and co-clique size M is*

$$\{\ (M + N)^{(N)}, N^{(M-1)}, 0^{(1)}\ \},$$

where $P^{(Q)}$ denotes Q copies of the number P. The eigenspace corresponding to the eigenvalue N consists of all vectors of the form $\begin{pmatrix} \mathbf{0}_N \\ v \end{pmatrix}$, where v is M-dimensional and $v \perp \mathbf{1}_M$; the eigenspace corresponding to the eigenvalue $(M+N)$ is spanned by the orthogonal vectors

$$(\mathbf{0}_{i-1},\ M+N-i,\ -\mathbf{1}_{M+N-i})^T, \quad 1 \le i \le N.$$

Lemma 8. *If $\lambda_N(G) > N$ or $\lambda_N(G) = N > \delta(G)$, then*

$$\lambda_{N+1}^{(\alpha)} \le N < \lambda_N^{(\alpha)} \text{ for all } 0 \le \alpha < 1.$$

Proof. We again make use of the Courant-Fischer-Weyl Min-Max Principle. Recall that the M-dimensional subspace $Q \subset \mathbb{R}^{M+N}$ consists of all vectors of the form $\begin{pmatrix} \mathbf{0}_N \\ u \end{pmatrix}$ with $u \in \mathbb{R}^M$. Then for any unit vector u,

$$\begin{aligned} \left\langle L_\alpha \begin{pmatrix} \mathbf{0}_N \\ u \end{pmatrix}, \begin{pmatrix} \mathbf{0}_N \\ u \end{pmatrix} \right\rangle &= (1-\alpha)\langle Nu, u\rangle + \alpha\langle D_1(u), u\rangle \\ &\le (1-\alpha)N + \alpha\delta(G) \le N. \end{aligned}$$

Therefore, the $(N+1)$-th largest eigenvalue $\lambda_{N+1}^{(\alpha)}$ is at most N.

For the eigenvalue $\lambda_N^{(\alpha)}$, let $\tilde{P}$ be the N-dimensional subspace which is spanned by the eigenvectors of L_1 corresponding to the N largest eigenvalues. Clearly $\tilde{P} \perp \mathbf{1}_{M+N}$. For any unit vector $v \in \tilde{P}$, we know from Lemma 7 that $\langle L_0(v), v\rangle \ge N$. Moreover,

$$\begin{aligned} \langle L_\alpha(v), v\rangle &= \alpha\langle L_1(v), v\rangle + (1-\alpha)\langle L_0(v), v\rangle \\ &\ge \alpha\,\lambda_N(G) + (1-\alpha)N \ge N. \end{aligned}$$

Therefore, the N-th largest eigenvalue $\lambda_N^{(\alpha)}$ is at least N.

We next proceed to show that the inequality on $\lambda_N^{(\alpha)}$ is strict when $0 \le \alpha < 1$. We already know that $\lambda_N^{(0)} = M+N$. If $\lambda_N^{(\alpha)} = N$ for some $0 < \alpha < 1$, then the above arguments show that necessarily

$$\lambda_N(G) = N, \quad \langle L_1 v, v\rangle = N, \text{ and } L_0(v) = Nv.$$

The first condition $\lambda_N(G) = N$ implies that $\delta(G) < N$, from our assumption on $\lambda_N(G)$; the third condition $L_0(v) = Nv$ implies that v is a unit vector in $\mathrm{Ker}(L_0 - N)$, thus in turn a unit vector of Q. Then

$$\langle L_1 v, v\rangle \le \delta(G) < N,$$

which contradicts the second condition $\langle L_1 v, v\rangle = N$. □

We now consider all possible N-dimensional subspaces $\begin{pmatrix} I_N \\ V^{(\alpha)} \end{pmatrix} \subseteq (\mathbf{1}_{M+N})^\perp$, where $V^{(\alpha)}$ is an $M \times N$ matrix. Here the notation of the subspace means that the subspace is spanned by the column vectors of the matrix $\begin{pmatrix} I_N \\ V^{(\alpha)} \end{pmatrix}$.

Lemma 9. *If the subspace* $\begin{pmatrix} I_N \\ V^{(\alpha)} \end{pmatrix} \subseteq (\mathbf{1}_{M+N})^{\perp}$ *is an invariant subspace of* L_α*, then the matrix* $V^{(\alpha)}$ *solves the quadratic matrix equation*

$$\begin{aligned} & V^{(\alpha)}\left[(1-\alpha)M + \alpha(N + D_1)\right] \\ =& -(1-\alpha)J_{M\times N} - \alpha A^T + \alpha\left[D_2 - V^{(\alpha)}(J_{N\times M} - A)\right]V^{(\alpha)}. \end{aligned}$$

In terms of matrix entries, this means that

$$v_{ji}^{(\alpha)} = \frac{-(1-\alpha) - \alpha\chi(i\sim j) + \alpha\left(f_j v_{ji} - \sum_{i'=1}^{N}\sum_{j'\nsim i'} v_{ji'}^{(\alpha)} v_{j'i}^{(\alpha)}\right)}{(1-\alpha)M + \alpha(N + d_i)}, \tag{1}$$

where the non-negative integers d_i*,* f_j *are the entries of the diagonal matrices*

$$D_1 = \mathrm{Diag}(d_1, d_2, \ldots, d_N), \quad D_2 = \mathrm{Diag}(f_1, f_2, \ldots, f_M).$$

Proof. It is easy to see that the orthogonal complement in $\mathbb{R}^{M+N}$ of the subspace $\begin{pmatrix} I_N \\ V^{(\alpha)} \end{pmatrix}$ is the subspace $\begin{pmatrix} -{V^{(\alpha)}}^T \\ I_M \end{pmatrix}$. If the subspace $\begin{pmatrix} I_N \\ V^{(\alpha)} \end{pmatrix}$ is an invariant subspace of L_α, then so is its orthogonal complement, since L_α is a symmetric matrix.

The L_α-invariance property is equivalent to the existence of two square matrices X_α and Y_α such that

$$L_\alpha \begin{pmatrix} I_N & -{V^{(\alpha)}}^T \\ V^{(\alpha)} & I_M \end{pmatrix} = \begin{pmatrix} I_N & -{V^{(\alpha)}}^T \\ V^{(\alpha)} & I_M \end{pmatrix}\begin{pmatrix} X_\alpha & 0 \\ 0 & Y_\alpha \end{pmatrix}.$$

By comparison of the corresponding four block matrices, we immediately obtain that

$$\begin{aligned} X_\alpha &= K_N + (1-\alpha)M + \alpha D_1 - [(1-\alpha)J_{N\times M} + \alpha A]V^{(\alpha)}, \\ Y_\alpha &= (1-\alpha)N + \alpha D_2 + [(1-\alpha)J_{M\times N} + \alpha A^T]{V^{(\alpha)}}^T, \end{aligned}$$

together with a quadratic matrix equation for $V^{(\alpha)}$:

$$\begin{aligned} & V^{(\alpha)}\left[K_N + (1-\alpha)M + \alpha D_1\right] + (1-\alpha)J_{M\times N} + \alpha A^T \\ =& \left\{(1-\alpha)N + \alpha D_2 + V^{(\alpha)}\left[(1-\alpha)J_{N\times M} + \alpha A\right]\right\}V^{(\alpha)}. \end{aligned}$$

Because $\begin{pmatrix} I_N \\ V^{(\alpha)} \end{pmatrix} \perp \mathbf{1}_{M+N}$, the entries of $V^{(\alpha)}$ satisfy that

$$\sum_{j=1}^{M} v_{ji}^{(\alpha)} = -1 \text{ for any } 1 \le i \le N.$$

This condition, in terms of matrices, is equivalent to $J_{N\times M}V^{(\alpha)} = -J_{N\times N}$. This implies that $V^{(\alpha)}K_N = [N + V^{(\alpha)}J_{N\times M}]V^{(\alpha)}$, with which the above quadratic matrix equation can be simplified to

$$\begin{aligned} & V^{(\alpha)}[(1-\alpha)M + \alpha(N + D_1)] \\ =& -(1-\alpha)J_{M\times N} - \alpha A^T + \alpha\left[D_2 - V^{(\alpha)}(J_{N\times M} - A)\right]V^{(\alpha)}. \qquad \square \end{aligned}$$

The quadratic matrix equation is complicated, and is almost impossible to be solved explicitly. Fortunately, we do not have to do so.

From Lemma 8 and the assumption on $\lambda_N(G)$, we know that

$$\lambda_{N+1}^{(\alpha)} \lneqq \lambda_N^{(\alpha)} \quad \text{for all} \quad \alpha \in [0,1].$$

Thus the subspace spanned by the eigenvectors of L_α corresponding to the N largest eigenvalues is unique. Assume that this subspace is given by $\begin{pmatrix} I_N \\ V^{(\alpha)} \end{pmatrix}$, so that the matrix $V^{(\alpha)}$ is well defined.

Lemma 10. *The map $V^{(\alpha)} : [0,1] \to \mathbb{R}^{M\times N}$ is a continuous function of α, for the usual metric of $\mathbb{R}^{M\times N}$.*

Proof. Assume that α_n is a sequence in $[0,1]$ such that $\alpha_n \to \alpha$ as $n \to \infty$.

According to the algebraic multiplicity of eigenvalues of L_α, there exist positive integers $l = l(\alpha)$ and $i_1, \dots, i_l$ ($i_0 = 0$ by convention) such that $i_1 + i_2 + \cdots + i_l = N$ and

$$\lambda_{i_1+\cdots+i_{k-1}+1}^{(\alpha)} = \cdots = \lambda_{i_1+\cdots+i_{k-1}+i_k}^{(\alpha)} > \lambda_{1+i_1+\cdots+i_{k-1}+i_k}^{(\alpha)}, \quad \forall 1 \le k \le l.$$

Let $\{u_i^\beta\}_{i=1}^{M+N}$ be an orthonormal basis consisting of the eigenvectors corresponding to the eigenvalues $\lambda_i^{(\beta)}$ for any $\beta \in [0,1]$, and $\{Z_k^{\alpha_n}\}_{k=1}^l$, $\{W_k^\alpha\}_{k=1}^l$ denote two sequences of monotonic subspaces of $\mathbb{R}^{M+N}$ given by

$$Z_k^{\alpha_n} = \operatorname{span}\{u_i^{\alpha_n} : i \le i_1 + \cdots + i_k\},\ W_k^\alpha = \operatorname{span}\{u_i^\alpha : i > i_1 + \cdots + i_{k-1}\}.$$

By the Courant-Fischer-Weyl Min-Max Principle,

$$\min_{0\ne u\in Z_k^{\alpha_n}} \frac{\langle L_{\alpha_n}(u), u\rangle}{\langle u, u\rangle} = \lambda_{i_1+\cdots+i_k}^{(\alpha_n)} \to \lambda_{i_1+\cdots+i_k}^{(\alpha)} \quad \text{as } n \to \infty$$

and

$$\max_{0\ne v\in W_{k+1}^\alpha} \frac{\langle L_\alpha(v), v\rangle}{\langle v, v\rangle} = \lambda_{1+i_1+\cdots+i_k}^{(\alpha)} \lneqq \lambda_{i_1+\cdots+i_k}^{(\alpha)}.$$

It follows that $Z_k^{\alpha_n} \cap W_{k+1}^\alpha = \{0\}$ and $Z_k^{\alpha_n} \oplus W_{k+1}^\alpha = \mathbb{R}^{M+N}$ when n is sufficiently large. Moreover, we obtain that $Z_l^{\alpha_n} = \bigoplus_{k=1}^l (Z_k^{\alpha_n} \cap W_k^\alpha)$ from

$$\dim(Z_k^{\alpha_n} \cap W_k^\alpha) = \dim(Z_k^{\alpha_n}) + \dim(W_k^\alpha) - (M+N) = i_k.$$

Consider a basis of the subspace $Z_k^{\alpha_n} \cap W_k^\alpha$ which consists of unit vectors of the form

$$u_{k,n,s} = \cos(\theta_{k,n,s}) u_{i_1+\cdots+i_{k-1}+s}^\alpha + \sin(\theta_{k,n,s}) w_{k,s}, \quad 1 \le s \le i_k,$$

for some unit vector $w_{k,s} \in W_{k+1}^\alpha$. Necessarily $\lim_{n\to\infty} \sin(\theta_{k,n,s}) = 0$, since $\langle L_{\alpha_n}(u_{k,n,s}), u_{k,n,s}\rangle \ge \lambda_{i_1+\cdots+i_k}^{(\alpha_n)}$ and

$$\begin{aligned}\langle L_\alpha(u_{k,n,s}), u_{k,n,s}\rangle &= \cos^2(\theta_{k,n,s}) \lambda_{i_1+\cdots+i_k}^\alpha + \sin^2(\theta_{k,n,s}) \langle L_\alpha(w_{k,s}), w_{k,s}\rangle \\ &\le \cos^2(\theta_{k,n,s}) \lambda_{i_1+\cdots+i_k}^{(\alpha)} + \sin^2(\theta_{k,n,s}) \lambda_{i_1+\cdots+i_k+1}^{(\alpha)}.\end{aligned}$$

Any vector $u \in Z_l^{\alpha_n}$ can now be expressed as

$$u = \sum_{k=1}^l \sum_{s=1}^{i_k} c_{k,s} \left[\cos(\theta_{k,n,s}) u_{i_1+\cdots+i_{k-1}+s}^\alpha + \sin(\theta_{k,n,s}) w_{k,s}\right].$$

Assume that the maximum of $|c_{k,s}|$ is achieved at $|c_{k_0,s_0}|$. Due to the orthogonality of $\{u_i^\alpha\}_i$, the absolute value of the coefficient of $u^\alpha_{i_1+\cdots+i_{k_0-1}+s_0}$ is at most $\|u\|$. But when n is sufficiently large, it is at least

$$|c_{k_0,s_0}|\cdot\left(|\cos(\theta_{k_0,n,s_0})|-\sum_{k=1}^{l}\sum_{s=1}^{i_k}|\sin(\theta_{k,n,s})|\right)\geq\frac{|c_{k_0,s_0}|}{2}.$$

Hence $|c_{k_0,s_0}|\leq 2\|u\|$. For any given vector $v\in W^\alpha_{l+1}$, we see that

$$|\langle u,v\rangle|=\left|\sum_{k=1}^{l}\sum_{s=1}^{i_k}\langle c_{k,s}\sin(\theta_{k,n,s})w_{k,s},v\rangle\right|\leq 2\|u\|\cdot\|v\|\cdot\sum_{k=1}^{l}\sum_{s=1}^{i_k}|\sin(\theta_{k,n,s})|,$$

which goes to zero as n goes to infinity.

The subspace $Z_l^{\alpha_n}$ is nothing else but $\begin{pmatrix} I_N \\ V^{(\alpha_n)}\end{pmatrix}$, while W^α_{l+1} is nothing else but $\begin{pmatrix} -V^{(\alpha)^T} \\ I_M\end{pmatrix}$. The inner product of the i-th column vector of the first matrix and the j-th column vector of the second matrix is equal to

$$V_{ji}^{(\alpha_n)}-V_{ji}^{(\alpha)},$$

which must go to zero as n goes to infinity. This proves the continuity of $V^{(\alpha)}$ on α. □

Lemma 11. *Let Ω be the subset*

$$\{(x_{ji}):\sum_{k=1}^{M}x_{ki}=-1,\ \forall 1\leq i\leq N,\ \textit{and}\ \ x_{ji}\leq 0,\ \ \forall 1\leq j\leq M, 1\leq i\leq N\}$$

of $\mathbb{R}^{M\times N}$. Then $V^{(\alpha)}\in\Omega$ for all $\alpha\in[0,1]$.

Proof. Consider the subset

$$\Gamma=\{\alpha\in[0,1):V^{(\alpha)}\in\Omega\}$$

of the half-open half-closed interval $[0,1)$.

When $\alpha=0$, $v_{ji}^{(0)}\equiv-\frac{1}{M}$ (see Lemma 7 or equation (1)). As a consequence, $V^{(0)}\in\Omega$, so that $0\in\Gamma$ and Γ is not empty.

Suppose there is a sequence of points $\alpha_n\in\Gamma$ and $\lim_{n\to\infty}\alpha_n=\alpha$ with α still in $[0,1)$. By Lemma 10, $\lim_{n\to\infty}V^{(\alpha_n)}=V^{(\alpha)}$. Because Ω is a compact set, so $V^{(\alpha)}\in\Omega$ and $\alpha\in\Gamma$. Therefore, Γ is a closed subset of $[0,1)$.

Suppose $\alpha\in\Gamma$, namely $V^{(\alpha)}\in\Omega$ for some $\alpha\in[0,1)$. Because the quantities $\chi(i\sim j)$, f_j and $v_{ji'}^{(\alpha)}v_{j'i}^{(\alpha)}$ in equation (1) are all non-negative, we see that

$$v_{ji}^{(\alpha)}\leq\frac{-(1-\alpha)}{(1-\alpha)M+\alpha(N+d_i)}<0\text{ for all }1\leq j\leq M, 1\leq i\leq N.$$

Therefore $V^{(\alpha)}$ is contained in the interior of Ω. Since $V^{(\alpha)}$ depends continuously on α, it follows that Γ is an open subset of $[0,1)$.

The interval $[0,1)$ is connected, and Γ is an open closed non-empty subset of it, therefore Γ is equal to $[0,1)$.

By continuity at $\alpha=1$, $V^{(1)}$ is also in Ω. This proves that $V^{(\alpha)}\in\Omega$ for all $\alpha\in[0,1]$. □

During the proof of Lemma 9, we have already known that

$$L_\alpha \begin{pmatrix} I_N \\ V^{(\alpha)} \end{pmatrix} = \begin{pmatrix} I_N \\ V^{(\alpha)} \end{pmatrix} X_\alpha$$

where

$$X_\alpha = K_N + (1-\alpha)M + \alpha D_1 - [(1-\alpha)J_{N\times M} + \alpha A]V^{(\alpha)}.$$

So the sum of the N largest eigenvalues of L_1 is equal to the trace of

$$X_1 = K_N + D_1 - AV^{(1)}.$$

But $V^{(1)} \in \Omega$ by Lemma 11, therefore

$$\mathrm{Tr}(AV^{(1)}) = \sum_{i=1}^{N} \sum_{j:j\sim i} v_{ji} \geq \sum_{i=1}^{N} \sum_{j=1}^{M} v_{ji} = -N.$$

Then

$$\sum_{i=1}^{N} \lambda_i = N(N-1) + \mathrm{Tr}(D_1) - \mathrm{Tr}(AV^{(1)}) \leq N^2 + \mathrm{Tr}(D_1).$$

By Proposition 5, this completes the proof of Lemma 6.

4. Proof of the Grone-Merris Conjecture

For consistence we restate the Grone-Merris Conjecture here.

Grone-Merris Conjecture. For any graph G, its Laplacian spectrum is majorized by its conjugate degree sequence, namely $\lambda(G) \preccurlyeq \mathbf{d}'(G)$.

The Grone-Merris Conjecture behaves nicely under complementation, in the sense of the proposition below.

The *complement graph* of a graph G is a graph $\overline{G}$ on the same vertices such that two vertices of $\overline{G}$ are adjacent if and only if they are not adjacent in G. The Laplacian matrices of the graph G and of its complementary graph $\overline{G}$ are related by the property that

$$L(G) + L(\overline{G}) + J_n = nI_n.$$

All these matrices commute with each other, so that

$$\lambda(\overline{G}) = (n - \lambda_{n-1}(G), \ldots, n - \lambda_1(G), 0);$$
$$\mathbf{d}'(\overline{G}) = (n - d'_{n-1}(G), \ldots, n - d'_1(G), 0).$$

From these we see that

Proposition 12. *For any $1 \leq k < n$, the k-th inequality holds for the graph G if and only if the $(n-k-1)$-th inequality holds for the complement graph $\overline{G}$,*

$$\sum_{i=1}^{k} \lambda_i(G) \leq \sum_{i=1}^{k} d'_i(G) \Longleftrightarrow \sum_{j=1}^{n-1-k} \lambda_j(\overline{G}) \leq \sum_{j=1}^{n-1-k} d'_j(\overline{G}), \quad \forall 1 \leq k < n.$$

We are now ready to prove the Grone-Merris Conjecture.

Assume that the Grone-Merris Conjecture is not true, and the graph $G = (V, E)$ is a counterexample. Namely, there exists an integer k with $1 < k < n = |V|$, such that

$$\sum_{i=1}^{k} \lambda_i > \sum_{i=1}^{k} d'_i.$$

Without loss of generality, we can assume that this integer k is minimum over all counterexamples. Then we have

$$\sum_{i=1}^{k-1} \lambda_i \leq \sum_{i=1}^{k-1} d_i', \quad \text{and} \quad \lambda_k > d_k'.$$

Moreover, we can further assume that the number $|E|$ of edges is minimum over all counterexamples with the same k. Under this assumption, we claim that

Lemma 13. *For any two vertices i, j in the graph G, if $d_i \leq k$ and $d_j \leq k$, then they are not adjacent in G.*

Proof. We will prove this by contradiction by assuming that the lemma is false. Namely there exists a pair of vertices such that

$$d_i \leq k, \quad d_j \leq k, \quad i \sim j.$$

Let $\widetilde{G}$ be the graph obtained from G by deleting the edge ij. Due to the minimum property of $|E|$, we must have

$$\sum_{i=1}^{k} \lambda_i(\widetilde{G}) \leq \sum_{i=1}^{k} d_i'(\widetilde{G}).$$

Two Laplacian matrices are related via $L(G) = L(\widetilde{G}) + H$, where $H_{n\times n}$ is a positive semi-definite matrix whose only non-zero entries are $H_{ii} = H_{jj} = 1$ and $H_{ij} = H_{ji} = -1$. Applying Fan's Theorem 3, we see that

$$\begin{aligned} \sum_{i=1}^{k} \lambda_i(G) &\leq \sum_{i=1}^{k} \lambda_i(\widetilde{G}) + \sum_{i=1}^{k} \lambda_i(H) \leq \sum_{i=1}^{k} d_i'(\widetilde{G}) + Tr(H) \\ &= \left[\sum_{i=1}^{k} d_i'(G) - 2\right] + 2 = \sum_{i=1}^{k} d_i'(G). \end{aligned}$$

This contradicts our assumption that G was a counterexample, and therefore concludes the proof. $\square$

Next, we add new edges to G to get a new graph $\widehat{G}$. Add to G a new edge ij for any pair of vertices i, j in G such that

$$d_i \geq k, \ d_j \geq k, \ \text{and } i \nsim j.$$

The new graph $\widehat{G}$ so obtained is a split graph.

The clique of $\widehat{G}$ consists of all vertices of G whose degree is at least k, so the size of the clique is equal to $d_k'(G)$. Let $N = d_k'(G)$ denote this size. The co-clique consists of all vertices of G whose degree is less than k, so the maximum degree of vertices in the co-clique is $\delta(\widehat{G}) \leq k-1$.

Note that

$$d_1'(\widehat{G}) = d_1'(G), \ldots, d_k'(\widehat{G}) = d_k'(G)$$

while $\lambda_i(\widehat{G}) \geq \lambda_i(G)$ for all $1 \leq i \leq n$, so these two inequalities are still valid for the new graph $\widehat{G}$, namely

$$\sum_{i=1}^{k} \lambda_i(\widehat{G}) > \sum_{i=1}^{k} d_i'(\widehat{G}) \quad \text{and} \quad \lambda_k(\widehat{G}) > d_k'(\widehat{G}) = N.$$

Let us discuss the relationship between N and k.

If $N < k$, then $\lambda_k(\widehat{G}) \le \lambda_{N+1}(\widehat{G}) \le N$, which leads to a contradiction. The second inequality comes from Proposition 5.

If $N = k$, then $\widehat{G}$ is a split graph of clique size N, with the property that

$$\sum_{i=1}^{N} \lambda_i(\widehat{G}) > \sum_{i=1}^{N} d'_i(\widehat{G}) \quad \text{and} \quad \lambda_N(\widehat{G}) > N.$$

This contradicts Lemma 6.

So $k < N$. Note that $\widehat{G}$ is a split graph of clique size N. In this graph $\widehat{G}$, the maximum degree of vertices in the co-clique is at most $(k-1)$, while the minimum degree of vertices in the clique is at least $(N-1)$. This means that

$$d'_{N-1}(\widehat{G}) = \cdots = d'_{k+1}(\widehat{G}) = d'_k(\widehat{G}) = N.$$

Combining this with $\lambda_{k+1}(\widehat{G}) \ge \ldots \ge \lambda_{N-1}(\widehat{G}) \ge N$ from Proposition 5, we see immediately that the inequality

$$\sum_{i=1}^{k} \lambda_i(\widehat{G}) > \sum_{i=1}^{k} d'_i(\widehat{G}) \text{ can be extended to } \sum_{i=1}^{N-1} \lambda_i(\widehat{G}) > \sum_{i=1}^{N-1} d'_i(\widehat{G}).$$

Then we proceed to compare $\lambda_N(\widehat{G})$ with the clique size N.

First consider the case where $\lambda_N(\widehat{G}) \ge N$. Because $N = d'_{N-1}(\widehat{G}) \ge d'_N(\widehat{G})$, the split graph $\widehat{G}$ has clique size N, with the additional property that

$$\sum_{i=1}^{N} \lambda_i(\widehat{G}) > \sum_{i=1}^{N} d'_i(\widehat{G}) \quad \text{and} \quad \lambda_N(\widehat{G}) \ge N > \delta(\widehat{G}).$$

This again contradicts Lemma 6.

In the other case, where $\lambda_N(\widehat{G}) < N$, we switch attention to the complement graph of $\widehat{G}$. This complement graph is another split graph $\overline{\widehat{G}}$. Its clique size is M, and

$$\lambda_M(\overline{\widehat{G}}) = (N+M) - \lambda_N(\widehat{G}) > M.$$

According to Proposition 12,

$$\sum_{i=1}^{N-1} \lambda_i(\widehat{G}) > \sum_{i=1}^{N-1} d'_i(\widehat{G}) \quad \Longrightarrow \quad \sum_{i=1}^{M} \lambda_i(\overline{\widehat{G}}) > \sum_{i=1}^{M} d'_i(\overline{\widehat{G}}).$$

Therefore, $\overline{\widehat{G}}$ is a split graph of clique size M, with the additional property that

$$\sum_{i=1}^{M} \lambda_i(\overline{\widehat{G}}) > \sum_{i=1}^{M} d'_i(\overline{\widehat{G}}) \quad \text{and} \quad \lambda_M(\overline{\widehat{G}}) > M.$$

This again contradicts Lemma 6.

All possible cases are eliminated, and the Grone-Merris Conjecture is proved.

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