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Grone and Merris (5) conjectured that the Laplacian spectrum of a graph is majorized by its conjugate vertex degree sequence. We prove that this conjecture holds for a class of graphs including trees. We also show that this conjecture and its generalization to graphs with Dirichlet boundary conditions are equivalent.

Keywords: graph Laplacian, majorization, graph spectrum, degree sequence

1 Introduction

One way to extract information about the structure of a graph is to encode the graph in a matrix and study the invariants of that matrix, such as the spectrum. In this note, we study the spectrum of the Combinatorial Laplacian matrix of a graph.

The *Combinatorial Laplacian* of a simple graph $G = (V, E)$ on the set of n vertices is the $n \times n$ matrix $L(G)$ that records the vertex degrees on its diagonal and -1 when an off-diagonal entry ij corresponds to an edge (i, j) of G. The matrix $L(G)$ is positive semidefinite, so its eigenvalues are real and non-negative. We list them in non-increasing order and with multiplicity: $\lambda_1(G) \geq \lambda_2(G) \geq \ldots \geq \lambda_n(G) = 0$

We are interested in the conjecture of Grone and Merris (GM) that the spectrum $\lambda(L(G))$ is majorized by the conjugate partition of the non-increasing sequence of vertex degrees of G (5). This question is currently being studied (see for example (4)), but has yet to be resolved. We extend the class of graphs for which the conjecture is known to hold to include trees. We also show that if GM holds for graph Laplacians, it also holds for more general Dirichlet Laplacians (cf. (2)) as conjectured by Duval (3).

2 Background and definitions

Given a graph $G = (V, E)$ with $n = |V|$ vertices and $m = |E|$ edges, there are several ways to represent G as a matrix. There is the *edge–incidence matrix*, a $n \times m$ matrix that records in each column the two vertices incident on a given edge. For directed graphs we can consider a *signed* edge–incidence matrix $\partial(G)$ which records 1 for the head of an edge and -1 for the tail. There is also the $n \times n$ *adjacency matrix* $A(G)$ whose ijth entry is 1 when (i, j) is an edge of G, 0 otherwise.

We can encode the (vertex) degree sequence of G in non-increasing order as a vector $d(G)$ of length n, and in an $n \times n$ matrix $D(G)$ whose diagonal is $d(G)$ and whose off-diagonal elements are 0. Then the Combinatorial Laplacian $L(G)$ that we study is simply $D(G) - A(G)$. It is easy to check that if we (arbitrarily) orient G and consider the matrix $\partial(G)$ above, we also have $L(G) = \partial(G)\partial(G)^t$.

The field of spectral graph theory is the study of the structure of graphs through the spectra (eigenvalues) of matrices encoding G. For a survey see (1). Besides theoretical aspects of spectral graph theory, there are a wide range of applications of the subject to chemistry and physics as well as to problems in other branches of mathematics such as random walks and isoperimetric problems. In the case of $L(G)$, there has been considerable effort to study the eigenvalue λ_{n-1}, which is known as the *algebraic connectivity* of G. It can be shown that $\lambda_{n-1}(G) = 0$ if and only if G is disconnected. Bounds on $\lambda_{n-1}(G)$ give information on how well connected a graph is, and are useful, for example, in showing the existence of expander graphs. This and other applications are discussed in (1).

Currently, little is known about the middle terms of the spectrum. This is partly because it varies widely depending on the graph. However, Grone and Merris (5) conjecture that the conjugate partition of the degree sequence majorizes the spectrum, and showed that the majorization inequalities are tight on the class of *threshold* graphs. This conjecture has been extended to simplicial complexes in recent work by Duval and Reiner (4).

We recall that a *partition* $p = p(i)$ is a non-increasing sequence of natural numbers, and its *conjugate* is the sequence $p^T(j) := |\{i : p(i) \leq j\}|$. Then p^T has exactly $p(1)$ non-zero elements. When convenient, we can add or drop trailing zeros in a partition. For non-increasing real sequences s and t of length n, we say that s is *majorized* by t (denoted $s \trianglelefteq t$) if for all $k \leq n$: $\sum_{i=1}^{k} s_i \leq \sum_{i=1}^{k} t_i$ and $\sum_{i=1}^{n} s_i = \sum_{i=1}^{n} t_i$. The concept of majorization extends to vectors by comparing the non-increasing vectors produced by sorting the elements of the vector into non-increasing order.

There is a rich theory of majorization inequalities which occur throughout mathematics, see for example (6). Matrices are an important source of such inequalities. Notably, the relationship between the diagonal and spectrum of a Hermitian matrix is characterized by majorization. Many useful facts about majorization can be found in (6). We mention two in particular:

Fan's theorem is that for positive semidefinite matrices A and B: $\lambda(A + B) \trianglelefteq \lambda(A) + \lambda(B)$.

The Gale-Ryser theorem is as follows: Let A be an $m \times n$ 0-1 (or incidence) matrix, with row sums $r_1, \ldots, r_m$ and columns sums $c_1, \ldots, c_n$ both indexed in non-increasing order. Let r^T be the conjugate of the partition $(r_1, \ldots, r_m)$, and c be the partition $(c_1, \ldots, c_n)$. Then: $c \trianglelefteq r^T$.

The Grone-Merris conjecture (GM) is that the spectrum of the combinatorial Laplacian of a graph is majorized by its conjugate degree sequence, that is: $\lambda(G) \trianglelefteq d^T(G)$.

If we ignore isolated vertices (which contribute only zero entries to λ and d) we will have $d_1^T = n$. Using this fact, it is possible to show that $\lambda_1 \leq d_1^T$. Three short proofs of this are given in (4). The authors then continue to prove the second majorization inequality: $\lambda_1 + \lambda_2 \leq d_1^T + d_2^T$. However, their proof would be difficult to extend.

There are several other facts which fit well with the GM conjecture. One is that if the GM conjecture holds, then the instances where GM holds with equality are well-understood, these would be the threshold graphs (see below). Also, since d and λ are respectively the diagonal and spectrum of $L(G)$ we have $d \trianglelefteq \lambda$. Combining this with GM gives $d \trianglelefteq d^T$, a fact that has been proved combinatorially. We refer to (4) for further discussion.

3 Grone-Merris on classes of graphs

In this section we give further evidence for the Grone-Merris conjecture by remarking that it holds for several classes of graphs including threshold graphs, regular graphs and trees.

The GM conjecture was originally formulated in the context of *threshold* graphs, which are a class of graphs with several extremal properties. Threshold graphs are the graphs that can be constructed recursively by adding isolated vertices and taking graph complements. It turns out that they are also characterized by degree sequences: the convex hull of possible (unordered) degree sequences of an n vertex graph defines a polytope. The extreme points of this polytope are the degree sequences that have a unique labelled realization, and these realizations are exactly the threshold graphs.

Threshold graphs are interesting from the point of view of spectra. Several people, including Grone and Merris (5) have studied the question of which graphs have integer spectra. It turns out that threshold graphs are one class of graphs that have integer spectra, and for these graphs we have $\lambda(G) = d^T(G)$.

In the process of showing this equality for threshold graphs, Grone and Merris observed that for non-threshold graphs, the majorization inequality $\lambda(G) \trianglelefteq d^T(G)$ appears to hold, and made their conjecture. We could describe the conjecture as saying that threshold graphs are extreme in terms of spectra, and that these extreme spectra can be interpreted as conjugate degree sequences.

For some small classes of graphs, it can be easily shown that the GM conjecture holds. Consider a k-regular graph G on n vertices (in a k-*regular* graph, all vertices have degree k). Then the degree sequence $d(G)$ is k repeated n times, and its conjugate $d^T(G)$ is n repeated k times followed by $n-k$ zeros. Thus d^T majorizes every non-negative sequence of sum kn whose largest terms is at most n, and in particular $\lambda \trianglelefteq d^T$.

Using facts about the initial GM inequalities we can prove that GM must hold for graphs with low maximal degree. For example, if a graph has maximum vertex degree 2, then $d^T_3 = d^T_4 = \ldots = d^T_n = 0$, so for $k = 2, 3, \ldots, n$: $\sum_{i=1}^k \lambda_i \le \sum_{i=1}^n \lambda_i = \sum_{i=1}^n d^T_i = \sum_{i=1}^k d^T_i$. More generally, the GM inequalities for $k \ge \max\_\deg(G)$ hold trivially. Since $\lambda_1 \le d^T_1$ we get that GM holds for graphs of maximum degree 2. Using the second majorization inequality we see that GM holds for graphs of maximum degree 3.

It is tempting to try to prove GM inductively by breaking graphs into simpler components on which GM clearly holds. In this section, we remark that if G is almost the union of two smaller graphs on which GM holds then GM holds for G as well. In particular, this result implies that GM holds for trees.

Take two graphs $A = (V_A, E_A)$ and $B = (V_B, E_B)$ on disjoint vertex sets V_A and V_B. Define their *disjoint sum* to be $A + B = (V_A \cup V_B, E_A \cup E_B)$. Assuming V_A and V_B are not empty this is a disconnected graph. Now take two graphs $G = (V, E_G)$ and $H = (V, E_H)$ on the same vertex set V. Define their *union* as $G \cup H = (V, E_G \cup E_H)$.

Given the spectra and conjugate degree sequences of A and B, the spectrum of $A+B$ is (up to ordering) the concatenation of the vectors $\lambda(A)$ and $\lambda(B)$, while the conjugate degree sequence of $A+B$ is $d^T(A+B) = d^T(A) + d^T(B)$ (taking each vector to have length n). Then if $\lambda(A) \trianglelefteq d^T(A)$ and $\lambda(B) \trianglelefteq d^T(B)$ we will have $\lambda(A+B) \trianglelefteq d^T(A+B)$. In a typical situation, where neither A or B is very small, we would expect the above majorization inequality to hold with considerable slack. We can use this slack to show that if we add a few more edges to $A + B$ the majorization will still hold.

Theorem 3.1 *Take graphs A or B on disjoint vertex sets V_A and V_B. Let $G = A+B$ and on $V = V_A \cup V_B$ let C be a graph of "new edges" between V_A and V_B. Assume that GM holds on A, B and C, i.e. that $\lambda(A) \trianglelefteq d^T(A)$, $\lambda(B) \trianglelefteq d^T(B)$ and $\lambda(C) \trianglelefteq d^T(C)$. Additionally, assume that $d^T_i(C) \le d^T_i(A), d^T_i(B)$ for all i, and that $d^T_1(B) \le d^T_m(A)$ where m is the largest non-zero index of $d^T(C)$ (equivalently, m is the maximum vertex degree in C). Let $H = C \cup G$. Then: $\lambda(H) \trianglelefteq d^T(H)$.*

This theorem is proved by carefully estimating the slack in $\lambda(G) \trianglelefteq d^T(G)$, the details are omitted here. Theorem 3.1 implies that GM holds for trees by induction: trees of diameter 1 or 2 are threshold graphs, while trees of diameter at least 3 can be decomposed into two smaller trees A and B with at least one edge, and a single linking edge C.

4 Simplices and pairs

The most recent work relating to the GM conjecture has been to study the spectra of more general structures than graphs, such as simplicial complexes and simplicial family pairs. In this section we show that the generalization of GM to graphs with Dirichlet boundary conditions is equivalent to the original conjecture and may be useful in approaching GM.

In (4), the authors look at *simplicial complexes*, which are higher dimensional analogues of simple graphs. A set of faces of a given dimension i is called an *i-family*. Given a simplicial complex Δ we can denote the i-family of all faces in Δ of dimension i as $\Delta^{(i)}$. For example, a graph is a 1-dimensional complex, and its edge set is the 1-family $\Delta^{(1)}$. Define the degree sequence d of an i-family to be the list of the numbers of i-faces from the family incident on each vertex, and sorted into non-increasing order. We can then define $d(\Delta, i)$ as the degree sequence of $\Delta^{(i)}$, which we can abbreviate to $d(\Delta)$ or d when the context is clear.

We define the *chain group* $C_i(\Delta)$ of formal linear combinations of elements of $\Delta^{(i)}$, and generalize the signed incidence matrix ∂ of Section 2 to a signed boundary map $\partial_i : C_i(\Delta) \to C_{i-1}(\Delta)$. This allows us to define a *Laplacian* on $C_i(\Delta)$, namely $L_i(\Delta) = \partial_i \partial_i^T$, and study its corresponding spectrum $s(\Delta, i)$ sometimes abbreviated $s(\Delta)$ or s.

Duval and Reiner (4) looked at *shifted* simplicial complexes, which are a generalization of threshold graphs to complexes. They showed that for a shifted complex Δ and any i, we have $s(\Delta, i) = d^T(\Delta, i)$. They then conjectured that GM also holds for complexes, i.e. that for any complex and any i we have: $s(\Delta, i) \trianglelefteq d^T(\Delta, i)$ They also show that some related facts, such as $\lambda_1 \leq d_1^T$ generalize to complexes.

In (3), Duval continues by studying *relative (family) pairs* (K, K') where the set $K = \Delta^{(i)}$ for some i is taken modulo a family of $(i-1)$-faces $K' \subseteq \Delta^{(i-1)}$. When $K' = \emptyset$, this reduces to the situation of the previous section. In the case $i = 1$ this is the edge set of a graph (K) with a set of *deleted* boundary vertices K'. This type of graph with a boundary appears in conformal invariant theory. In this language, the relative Laplacian of an (edge, vertex) pair is sometimes referred to as a *Dirichlet Laplacian* and its eigenvalues as *Dirichlet eigenvalues*, see for example (2).

We can form chain groups $C_i(K)$ and $C_{i-1}(K, K')$ and use these to define a (signed) boundary operator on the pair $\partial(K, K') : C_i(K) \to C_{i-1}(K, K')$. Hence we get a Laplacian for family pairs $L(K, K') = \partial(K, K')\partial(K, K')^T$. Considered as a matrix, $L(K, K')$ will be the principal submatrix of $L(K)$ whose rows are indexed by the i-faces in $\Delta^{(i-1)} - K'$. Finally, we get a spectrum $s(K, K')$ for family pairs from the eigenvalues of $L(K, K')$.

Duval defines the degree $d_v(K, K')$ of vertex v (in the case of a graph, v is allowed to be in K') relative to the pair (K, K') as the number of faces in K that contain v such that $K - \{v\}$ is in $\Delta^{(i-1)} - K'$. This allows him to define the degree sequence $d(K, K')$ for pairs, and to conjecture that GM holds for relative pairs: $s(K, K') \trianglelefteq d^T(K, K')$.

It turns out that at least in the case of (edge, vertex) pairs this majorization follows from the original GM conjecture for graphs.

Theorem 4.1 *GM for graphs $\Rightarrow$ GM for (edge, vertex) pairs.*

Proof: Let $G = (V, E)$ be a graph with $D \subseteq V$ a set of "deleted" vertices. Let $U = V - D$ be the remaining undeleted vertices. We will assume that GM holds only on the undeleted part of the graph, i.e. $G|_U$. So we have $s(G|_U) \trianglelefteq d^T(G|_U)$. We can ignore the edges in $G|_D$ completely, since they have no effect on either $s(E, D)$ or $d(E, D)$. The remaining edges connect vertices in D to vertices in U. Define G' to be the graph on V whose edge are exactly the edges of G between D and U. Let a be the degree sequence of the deleted vertices in G' and b be the degree sequence of the undeleted vertices in G'.

We can compute $d^T(E, D)$ in terms of the degree sequences and spectra of $G|_U$, G' and $G|_D$ since $d_i^T(E, D)$ is the number of vertices (deleted or not) attached to at least i non-deleted vertices. The number of such vertices in U will be $d_i^T(G|_U)$, and the number in D will be $d_i^T(G') = a^T$. Hence $d^T(E, D) = d_i^T(G|_U) + a^T$.

Now consider the Laplacian $L(E, D)$. This is the submatrix of $L(G)$ indexed by U. An edge (i, j) in $G|_U$ contributes to entries ii, ij, ji, jj in both $L(E, D)$ and $L(G)$. An edge in G', say from $i \in U$ to $j \in D$ contributes only to entry ii, and an edge in $G|_D$ does not affect $L(E, D)$. So, we have $L(E, D) = L(G|_U) + \mathrm{Diag}(b)$, and by Fan's theorem we have: $s(E, D) \trianglelefteq s(G|_U) + b$.

We complete our equivalence by appealing to the Gale-Ryser theorem to claim that $b \trianglelefteq a^T$. This follows from the fact that a and b are row and column sums (in non-increasing order) of the $|D| \times |U|$ bipartite incidence matrix for G'. Combining this with the majorization above and the assumption that $s(G|_U) \trianglelefteq d^T(G|_U)$ we get: $s(E, D) \trianglelefteq s(G|_U) + b \trianglelefteq d^T(G|_U) + a^T = d^T(E, D)$.

This proof relies on the bipartite structure of G', so it is not immediately obvious how to extend it to higher dimensional complexes. It would be interesting to do this.

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