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Threshold graphs of maximal Laplacian energy

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ABSTRACT

The Laplacian energy of a graph is defined as the sum of the absolute values of the differences of average degree and eigenvalues of the Laplacian matrix of the graph. This spectral graph parameter is upper bounded by the energy obtained when replacing the eigenvalues with the conjugate degree sequence of the graph, in which the ith number counts the nodes having degree at least i. Because the sequences of eigenvalues and conjugate degrees coincide for the class of threshold graphs, these are considered likely candidates for maximizing the Laplacian energy over all graphs with given number of nodes. We do not answer this open problem, but within the class of threshold graphs we give an explicit and constructive description of threshold graphs maximizing this spectral graph parameter for a given number of nodes, for given numbers of nodes and edges, and for given numbers of nodes, edges and trace of the conjugate degree sequence in the general as well as in the connected case. In particular this positively answers the conjecture that the pineapple maximizes the Laplacian energy over all connected threshold graphs with given number of nodes.

1. Introduction

For a simple undirected graph G on n nodes, consider the Laplacian matrix $L_G = D - A$, where A is the adjacency matrix of G and D is the diagonal degree matrix. The spectral parameter

$$\mathrm{LE}(G) = \sum_{i=1}^{n} |\lambda_i(L_G) - \bar{\delta}|,$$

where $\lambda_i(L_G)$ are the eigenvalues of L_G and $\bar{\delta}$ is the average degree, has been defined by Gutman and Zhou [4] as the *Laplacian energy* of G and it has been extensively studied since then.

Finding the graph on n nodes with largest Laplacian energy is a natural extremal problem in the area of spectral graph theory and has been considered before. In [3] it has been proved that the star S_n is the tree with largest Laplacian energy. For general graphs, in [2], we read "There was a conjecture that maximum Laplacian energy was obtained by a special class of threshold graphs called pineapples. A disconnected counterexample was discovered but the conjecture remains open for connected graphs. The (strict) upper bound of $2m$ (m is the number of edges) was obtained for Laplacian energy. Many related questions were posed and discussed concerning this hard topic".

Threshold graphs appear in many applications (see [5] for an account) but its connection with high Laplacian energy may be explained as follows (see the next section for definitions). For the graph G with degree sequence d and conjugate degree

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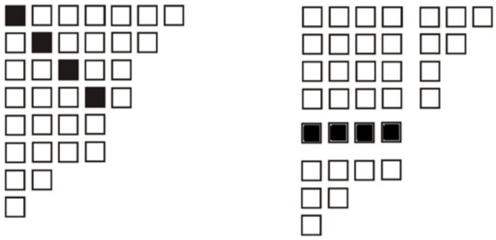

Fig. 1. Ferrers diagram of a threshold graph.

sequence d^*, the Grone–Merris conjecture, proved by Bai [1], states that the sequence of Laplacian eigenvalues is majorized by the sequence d^*, implying that

$$\mathrm{LE}(G) \leq \sum_{i=1}^{n} |d_i^* - \bar{\delta}|.$$

Since equality is attained by threshold graphs, it is natural to consider this class of graphs as good candidates for those having largest Laplacian energy.

In this paper we consider the problem of finding threshold graphs with maximal Laplacian energy. We find extremal graphs in this class fixing several parameters. First we determine optimal graphs for a fixed number of nodes, edges and trace. Then we find extremal graphs fixing the number of nodes and edges and finally we fix only the number of nodes.

Hence, in particular, we determine a threshold graph with highest Laplacian energy among those having n nodes. Indeed, we show that an extremal graph is a disconnected threshold graph with trace $f = \lfloor \frac{2n+1}{3} \rfloor$, $f(f+1)/2$ edges and whose Ferrers diagram is a rectangle $f(f+1)$. That is a clique of size $\lfloor \frac{2n+1}{3} \rfloor + 1$ together with $\lfloor \frac{n-2}{3} \rfloor$ isolated vertices. For connected threshold graphs, we show that the pineapple $P_{n,f'}$ with clique size $f'+1 = \lfloor \frac{2n}{3} \rfloor + 1$ has largest Laplacian energy among all connected threshold graphs with n vertices. This partially proves the conjecture posed in [8], giving further evidence that $P_{n,f'}$ is a connected graph on n vertices having largest Laplacian energy.

The paper is organized as follows. The next section introduces notions and definitions used throughout the paper. Then in Section 3 we determine threshold graphs, with fixed number of nodes, edges and trace, having largest Laplacian energy. We also show which one has largest Laplacian energy among those having fixed number of edges and nodes (dropping the fixed trace). In Section 4, studying the development of the energy when edges are added successively, we determine threshold graphs of maximum Laplacian energy among those having a fixed number of nodes. Finally, in the last section, we consider connected threshold graphs and prove that the pineapple $P_{n,f'}$ is extremal.

2. Degree sequences, threshold graphs and pineapples

Let $G = (V, E)$ be a simple undirected graph with node set $V = [n] := \{1, \dots, n\}$ for some $n \in \mathbb{N}$ and edge set $\emptyset \neq E \subseteq \binom{V}{2} := \{\{i,j\} : i, j \in V, i \neq j\}$. Denote by $m = |E|$ the number of edges and for $i \in V$ by $d_i := |\{j \in V : \{i,j\} \in E\}|$ the degree of node i. We assume throughout that the node numbering is such that degree sequences are non increasing, *i.e.* $d_1 \geq \cdots \geq d_n$. Any degree sequence $d \in \mathbb{N}_0^n$ arising this way is an n-partition of $2m$. For $i \in [n]$ the *conjugate degree sequence* is defined as $d_i^* := |\{j \in V : d_j \geq i\}|$, so $d_n^* = 0$. The conjugate degree sequence is conveniently visualized by means of Ferrers (or Young) diagrams, see [7]. For degree sequence $d \in \mathbb{N}_0^n$ it consists of n left justified rows of $\square$-symbols where row i holds d_i boxes. In this diagram, the conjugate degree d_i^* counts the number of boxes in column i. The diagonal width of the degree sequence $f = \max\{i \in V : d_i \geq i\}$ is called the *trace* of the partition. The square of $f \cdot f$ boxes in this diagram is called the *Durfee square* of the partition. For a given n-partition $d \in \mathbb{N}_0^n$ of $2m$ one can construct a graph having this degree sequence if and only if $\sum_{i=1}^{k} d_i \leq \sum_{i=1}^{k} (d_i^* - 1)$ for $k \in [f]$ (Ruch–Gutman Theorem, cf. [7]). Letting $\bar{\delta} = \frac{1}{n} \sum_{i \in V} d_i = \frac{2m}{n}$ denote the average degree of G, the Laplacian energy is defined as $\mathrm{LE}(G) = \sum_{i \in [n]} |\lambda_i(L_G) - \bar{\delta}|$.

Threshold graphs. G is called a threshold graph if $d_i = d_i^* - 1$ for $i \in [f]$. Geometrically, G is a threshold graph of trace f if and only if its Ferrers diagram can be decomposed into: its Durfee square; a row of f boxes directly below the Durfee square, darkened on the right of Fig. 1; and two remaining boxes placed in such a way that the shape below row $f+1$ has the transpose shape to the right of the Durfee square.

Note that the degree sequence of threshold graphs uniquely defines the graph itself (see, for example, [7]) and additionally, it is fully specified once the conjugate degrees d_i^* are given for $i \in [f]$. This will be exploited heavily and is easily seen by looking at a Ferrers diagram. There the part strictly below the diagonal boxes is the transpose of the part above and including the diagonal. Fig. 1 is the Ferrers diagram of the (threshold) graph given by the degree sequence $d = (7, 6, 5, 5, 4, 4, 2, 1)$. On the left, we emphasized the characterization given in this paragraph, darkening the diagonal boxes, whereas the right hand side illustrates the general appearance of a threshold graph based on the Durfee square visualization, described in the previous paragraph.