Threshold Graphs of Maximal Laplacian Energy

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The Laplacian energy of a graph sums up the absolute values of the differences of average degree and eigenvalues of the Laplace 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 i-th 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.

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MSC 2010: 05C50, 05C35

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.

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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 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. 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 $\mathrm{LE}(G) = \sum_{i \in [n]} |\lambda_i(L_G) - \bar{\delta}|$.

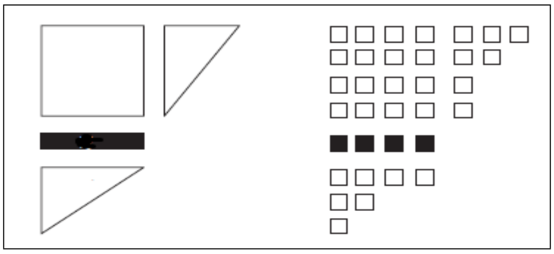

Figure 1: Ferrers diagram of a threshold graph.

Threshold Graphs. G is called a threshold graph if $d_i = d_i^* - 1$ for $i \in [f]$. Note that the degree sequence of threshold graphs 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. The right hand side of Figure 1 is the Ferrers diagram of the (threshold) graph given by the degree sequence $d = (7, 6, 5, 5, 4, 4, 2, 1)$, whereas the left hand side illustrates the general appearance of a threshold graph.

A pineapple $P_{n,f}$ is an n node graph composed by a clique of size $f+1$ and the remaining $n - f - 1$ vertices are all adjacent to a single vertex of the clique. It is easy to see that $P_{n,f}$ is a threshold graph of trace f. As an example, Figure 2 shows on the right hand side the pineapple $P_{13,5}$ and on the left hand side its Ferrers diagram. For a fixed number n of nodes, we can construct $n - 1$ pineapples by varying the trace from 1 (a star) to $n - 1$ (a complete graph). In [8] it has been shown that among all pineapples with n nodes, the Pineapple $P_{n,f'}$, $f' = \lfloor \frac{2n}{3} \rfloor$, has largest Laplacian energy. In this paper we show that $P_{n,f'}$ is the extremal graph among all connected threshold graphs with n nodes.

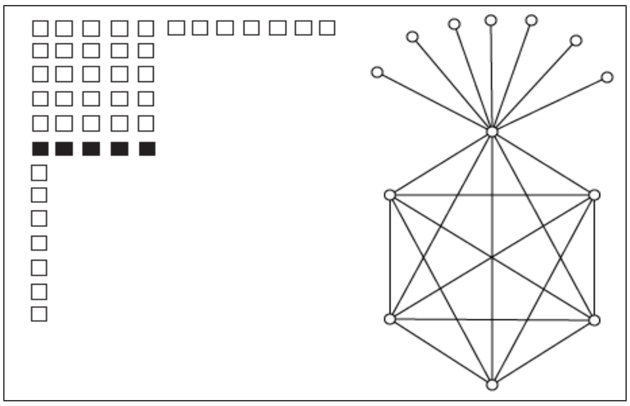

Figure 2: The pineapple $P_{13,5}$.

For n nodes and m edges the feasible range of traces f is determined by the constraints

$$f(f+1) \leq 2m \quad \text{and} \quad f(f+1) + 2(n-1-f)f = -f^2 + (2n-1)f \geq 2m.$$

Thus,

$$\underline{f}(n,m) := \left\lceil n - \frac{1}{2} - \sqrt{n^2 - n + \frac{1}{4} - 2m} \right\rceil \le f \le \left\lfloor -\frac{1}{2} + \sqrt{2m + \frac{1}{4}} \right\rfloor =: \bar{f}(m).$$

If n and m are clear from the context, we use $\underline{f}$ and $\bar{f}$ without their arguments. We will denote the threshold graph induced by a suitable conjugate degree sequence $d^* \in \mathbb{N}_0^n$ by $\mathrm{Th}^*(d^*)$.

In a threshold graph G its conjugate degree sequence d^* gives the spectrum of the Laplace matrix L_G, in particular $0 = \lambda_1(L_G) = d_n^* \le \lambda_2(L_G) = d_{n-1}^* \le \cdots \le \lambda_n(L_G) = d_1^*$, see [6]. Thus, for any threshold graph G we have

$$\mathrm{LE}(G) = \sum_{i\in[n]} |d_i^* - \bar{\delta}| = \sum_{d_i^* > \bar{\delta}} (d_i^* - \bar{\delta}) + \sum_{d_i^* \le \bar{\delta}} (\bar{\delta} - d_i^*).$$

By $\sum_{i\in[n]} d_i^* = 2m$ we have $\sum_{i\in[n]}(d_i^* - \bar{\delta}) = 0$ or $\sum_{d_i^* \ge \bar{\delta}}(d_i^* - \bar{\delta}) = \sum_{d_i^* \le \bar{\delta}}(\bar{\delta} - d_i^*)$, so

$$\mathrm{LE}(G) = 2 \sum_{d_i^* \ge \bar{\delta}} (d_i^* - \bar{\delta}) = 2 \sum_{d_i^* \le \bar{\delta}} (\bar{\delta} - d_i^*). \tag{1}$$

Our aim is to determine which threshold graphs are candidates for having maximal Laplacian energy for given n and m. Treating the general case first will also pave the way for the case of connected threshold graphs. Indeed, connected threshold graphs have $d_1^* = n$, so node 1 is connected to all other vertices. Thus, by "ignoring" this first node and the corresponding first column and row in its Ferrers diagram, the connected case can be reduced to the same procedure used for the solution of the general case.

3 Maximal energy for fixed number of nodes and edges

We first consider threshold graphs with fixed n, m and f and observe that within this group of threshold graphs a specific optimizer can be given explicitly. We explain the construction of the Ferrers diagram of the candidate graphs.

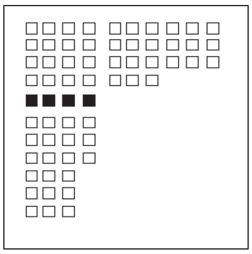

Figure 3: Type I threshold graph for $(n,m,f) = (11,31,4)$.

We call *Type I* the threshold graph with n vertices, m edges and trace f constructed in such a way that its conjugate degree sequence d^* is lexicographically maximal. In the following algorithmic construction of such a sequence it suffices to describe the placement of the m $\square$-symbols below the diagonal, because for threshold graphs the other m $\square$-symbols have to be placed on and above the diagonal in the corresponding transposed positions. In order to obtain a sequence with trace f, below the diagonal the first rows up to row $f+1$ have to be filled with $\square$-symbols (positions (i,j) for $1 \le j < i \le f+1$), then the remaining $m - f(f+1)/2$ $\Box$-symbols are placed in column-wise order, i.e., in the sequence $(f+2,1),(f+3,1),\ldots,(n,1),(f+2,2),(f+3,2),\ldots$. Figure 3 illustrates a Type I threshold graph with $n = 11$, $m = 31$ and $f = 4$. The conjugate degree sequence is $d^* = (11,11,11,8,4,4,4,3,3,3,0)$

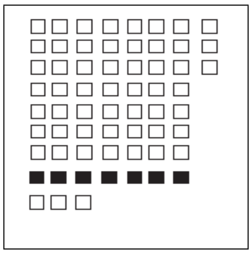

Figure 4: Type II threshold graph for $(n,m,f) = (11,31,7)$.

We call *Type II* the threshold graph with n vertices, m edges and trace f constructed in such a way that its conjugate degree sequence d^* is lexicographically minimal. A procedure to construct such a graph is to now to fill the positions on and above the diagonal in column-wise order without exceeding row index f, *i. e.*, the sequence reads $(1,1),(1,2),(2,2),(1,3),\ldots,(f,f),(1,f+1),\ldots,(f,f+1),(1,f+2),\ldots$ until m $\Box$-symbols have been placed (the corresponding m $\Box$-symbols below the diagonal need to be placed in row-wise order without exceeding column f). Figure 4 illustrates a Type II threshold graph with $n = 11$, $m = 31$ and $f = 7$. We notice that the conjugate degree sequence is $d^* = (9,9,9,8,8,8,8,3,0,0,0)$.

Lemma 1 *Among all threshold graphs on n nodes and m edges having a degree sequence with trace f the following are among those with maximal Laplacian energy:*

1. *for $f+1 \leq \bar{\delta}$ the Type I graph* i. e. *with $k = \left\lfloor \frac{m-f(f+1)/2}{n-1-f} \right\rfloor$ $(\leq f)$ its first f conjugate degrees are $d^*_i = n$ for $i \in [k]$, $d^*_i = f+1$ for $i \in \{k+2,\ldots,f\}$ and, if $k < f$, $d^*_{k+1} = f+1+m-f(f+1)/2-k(n-1-f)$,*
2. *for $f+1 \geq \bar{\delta}$ the Type II graph* i. e. *with $h = \left\lfloor \frac{m-f(f+1)/2}{f} \right\rfloor$ and $k = m-f(f+1)/2-fh$ $(\leq f)$ its first f conjugate degrees are $d^*_i = f+h+2$ for $i \in [k]$ and $d^*_i = f+h+1$ for $i \in \{k+1,\ldots,f\}$.*

Proof Case 1: Using Ferrers diagrams it can be worked out that the given conjugate degree sequence d^* has indeed trace f and belongs to a threshold graph G on n nodes and m edges. Now consider all threshold graphs on n nodes and m edges with degree sequence of trace f that have maximal Laplacian energy. Assume, for contradiction, that G is not in this set. Among the maximizers pick $\hat{G}$ with degree sequence $\hat{d}$ so that the largest index $i \in [f]$ with $\hat{d}^*_i > d^*_i$ is minimal and $\hat{d}^*_i - d^*_i$ is minimal as well. Let $\bar{\imath}$ be the corresponding index. Because d^* is lexicographically maximal, there must be an index $\hat{\imath} < \bar{\imath}$ with $d^*_{\hat{\imath}} > \hat{d}^*_{\hat{\imath}}$. Furthermore we may assume that either $\hat{\imath} = 1$ or $\hat{d}^*_{\hat{\imath}-1} > \hat{d}^*_{\hat{\imath}}$ by decreasing $\hat{\imath}$ otherwise. Now consider the conjugate degree sequence $\tilde{d}^*$ of a threshold graph defined via its first f elements by

$$\tilde{d}^*_i = \begin{cases} \hat{d}^*_i & i \in [f] \setminus \{\hat{\imath},\bar{\imath}\}, \\ \hat{d}^*_i + 1 & i = \hat{\imath}, \\ \hat{d}^*_i - 1 & i = \bar{\imath}. \end{cases}$$

The corresponding graph $\tilde{G}$ is again a threshold graph on n nodes and m edges having a degree sequence of trace f. It remains to show that the Laplacian energy $\mathrm{LE}(\tilde{G}) = 2\sum_{\tilde{d}_i^*\geq\bar{\delta}}(\tilde{d}_i^* - \bar{\delta})$ is at least as large as that of $\hat{G}$, then by the choice of $\hat{G}$ this yields the desired contradiction. For analyzing the change in energy we only need to consider the changes in the conjugate degrees with indices in $[f]$, more precisely only in $\hat{\imath}$ and $\bar{\imath}$, because for $i \in [n] \setminus [f]$ we have $\tilde{d}_i^* \leq f < \bar{\delta}$ as well as $\hat{d}_i^* \leq f$. If $\tilde{d}_{\bar{\imath}}^* \geq \bar{\delta}$ then also $\hat{d}_{\hat{\imath}}^* \geq \hat{d}_{\bar{\imath}}^* \geq \bar{\delta}$, so both graphs have the same energy. We may thus assume $\tilde{d}_{\bar{\imath}}^* = \hat{d}_{\bar{\imath}}^* - 1 < \bar{\delta}$ in the following. If $\tilde{d}_{\hat{\imath}}^* \leq \bar{\delta}$ then again this results in the same energy so we may also assume $\tilde{d}_{\hat{\imath}}^* = \hat{d}_{\hat{\imath}}^* + 1 > \bar{\delta}$. If $\hat{d}_{\bar{\imath}}^* \leq \bar{\delta}$ then $\sum_{\tilde{d}_i^*\geq\bar{\delta}}(\tilde{d}_i^* - \bar{\delta}) = \sum_{\hat{d}_i^*\geq\bar{\delta}}(\hat{d}_i^* - \bar{\delta}) + \min\{1, \tilde{d}_{\hat{\imath}}^* - \bar{\delta}\}$ and the energy increases. So the remaining case is $\bar{\delta} < \hat{d}_{\bar{\imath}}^* < \bar{\delta}+1$ which leads to $\sum_{\tilde{d}_i^*\geq\bar{\delta}}(\tilde{d}_i^* - \bar{\delta}) = \sum_{\hat{d}_i^*\geq\bar{\delta}}(\hat{d}_i^* - \bar{\delta}) + 1 - (\hat{d}_{\bar{\imath}}^* - \bar{\delta})$, thus an increase in energy again.

Case 2: Here d^* corresponds to a lexicographically minimal conjugate degree sequence amongst all of trace f for n nodes and m edges, but on the index set $[n] \setminus [f]$ its completion via the Ferrers diagram is in fact lexicographically maximal. This time, shifting one unit from the largest index in $[n] \setminus [f]$ with larger value to a smaller one in $[n] \setminus [f]$ with smaller value will prove the result by analogous arguments. □

The next result shows that the lexicographically extremal conjugate degree sequences of trace $\underline{f}$ and $\bar{f}$ give rise to candidates for threshold graphs on n nodes and m edges of maximal Laplacian energy.

Theorem 2 *The set of threshold graphs on n nodes and m edges with maximal Laplacian Energy contains at least one of these: the Type I threshold graph of trace $\underline{f}$ or the Type II threshold graph with trace $\bar{f}$.*

Proof Let G be a threshold graph of maximal Laplacian energy on n nodes and m edges and denote the trace of its conjugate degree sequence d^* by f.

Suppose first $f + 1 < \bar{\delta}$. In this case we assume G to be selected so that its trace f is minimal among all optimal threshold graphs. According to Lemma 1 we may assume that the sequence d^* of G is lexicographically maximal. If $f = \underline{f}$ we are done, so suppose, for contradiction, that $f > \underline{f}$. Because d^* is lexicographically maximal with $f > \underline{f}$ we know $d_f^* = f + 1$, $d_{f+1}^* < f$ and there is a smallest index $\hat{\imath} \in [f-1]$ with $d_{\hat{\imath}}^* < n$. Define a new conjugate degree sequence $\hat{d}^*$ of a threshold graph $\hat{G}$ on n nodes and m edges with trace $f - 1$ via

$$\hat{d}_i^* = \begin{cases} d_i^* & i \in [f-1] \setminus \{\hat{\imath}\}, \\ d_i^* + 1 & i = \hat{\imath}. \end{cases}$$

Note that extending this sequence results in $\hat{d}_f^* = f - 1$. Like in the proof of Lemma 1 one checks that $\mathrm{LE}(\hat{G}) \geq \mathrm{LE}(G)$. Because the trace of $\hat{G}$ is smaller than that of G this yields the desired contradiction.

It remains to consider the case $f + 1 \geq \bar{\delta}$. This time we assume G to have maximal trace f among all optimal threshold graphs. By Lemma 1 its conjugate degree sequence d^* may be assumed to be lexicographically minimal. For $f = \bar{f}$ the claim holds, so assume, for contradiction, $f < \bar{f}$. This and lexicographic minimality of d^* ensure $d_f^* \geq f + 2$, $d_{f+1}^* = f$ and the existence of a maximal index $\hat{\imath} \in [f]$ with $d_{\hat{\imath}}^* \geq f + 3$. Therefore we may specify a threshold graph $\hat{G}$ on n nodes and m edges with trace $f + 1$ via the first $f + 1$ entries of its degree sequence $\hat{d}^*$ by

$$\tilde{d}_i^* = \begin{cases} d_i^* & i \in [f] \setminus \{\hat{\imath}\}, \\ d_i^* - 1 & i = \hat{\imath}, \\ d_i^* + 2 & i = f + 1. \end{cases}$$

Again it suffices to track the changes in order to prove $\mathrm{LE}(\hat{G}) \geq \mathrm{LE}(G)$ and because of the larger trace of $\hat{G}$ this establishes the desired contradiction. $\square$

With this we can work out rather explicit formulas for the Laplacian energy for each case with given n and m by using (1). For the Type I threshold graph $\underline{f}$ with lexicographic maximal conjugate degree sequence $\underline{d}^*$,

$$\underline{TE}(n,m) := \mathrm{LE}(\mathrm{Th}^*(\underline{d}^*)) = \begin{cases} 2\bar{\delta}(n-m) & 2m \leq n, \\ 2[(\underline{f}-1)(n-\bar{\delta}) + \max\{0, \underline{d}^*_{\underline{f}} - \bar{\delta}\}] & 2m \geq n, \end{cases} \tag{2}$$

with

$$\underline{d}^*_{\underline{f}} = \underline{f} + 1 + m - \underline{f}(\underline{f}+1)/2 - (\underline{f}-1)(n-1-\underline{f}).$$

The case of Type II threshold graph with trace $\bar{f}$ and lexicographic minimal conjugate degree sequence $\bar{d}^*$ reads

$$\overline{TE}(n,m) := \mathrm{LE}(\mathrm{Th}^*(\bar{d}^*)) = 2[(n-1-\bar{f})\bar{\delta} + \max\{0, \bar{\delta} - \bar{d}^*_{\bar{f}+1}\}] \tag{3}$$

with

$$\bar{d}^*_{\bar{f}+1} = m - \bar{f}(\bar{f}+1)/2.$$

4 Maximal energy for fixed number of nodes

In order to find, for a fixed number of nodes n, which m determines the threshold graph with largest Laplacian energy, we study the behavior of the Laplacian energy of Type I and Type II graphs as a function of m.

First consider, for increasing m, the development of $\underline{TE}(n,m)$, which corresponds to the lexicographically maximal case generated in Ferrers diagram by filling up the first $\underline{f}(n,m)$ columns below the diagonal in column-wise order. Observe that the same minimal trace $k = \underline{f}(n,m) \in [n-1]$ is obtained for

$$\underline{m}_k := k(k+1)/2 + (k-1)(n-1-k) \leq m \leq \underline{m}_{k+1} - 1.$$

For $k \in [n-2]$ and $\underline{m}_k \leq m < \underline{m}_{k+1} - 1$ the value $h = m - \underline{m}_k + k + 1$ gives the row index of the last $\square$-symbol in column k and increasing m by one results in appending a $\square$-symbol in row $h+1$ of column k. The change of the value of $\underline{TE}(n,m)$ with $\bar{\delta} = \frac{2m}{n}$ to $\underline{TE}(n,m+1)$ with $\bar{\delta}_+ = \frac{2(m+1)}{n}$ can now be traced by distinguishing the cases on whether this next $\square$-symbol is still below the imaginary line through $\bar{\delta}_+$, just crosses it or whether the previous box was already above it. This gives rise to a recurrence relation for $\underline{TE}(n,m)$ along columns that allows to conclude that the maximum value over all columns must be attained in $m = \underline{m}_{\underline{k}+1} - 1$ for $\underline{k} = \lfloor \frac{n}{3} + \frac{5}{6} \rfloor$.

Lemma 3 *Given $n \geq 2$ and $m \geq n/2$ so that $k = \underline{f}(n,m) \in [n-2]$ and*

$$\underline{m}_k = k(k+1)/2 + (k-1)(n-1-k) \leq m < \underline{m}_{k+1} - 1,$$

let $\bar{\delta} = \frac{2m}{n}$, $\bar{\delta}_+ = \frac{2m+2}{n}$ and $h = m - \underline{m}_k + k + 1$, then

$$\underline{TE}(n,m+1) = \underline{TE}(n,m) + \begin{cases} -4\frac{k-1}{n} & h+1 \leq \bar{\delta}_+, \\ -4\frac{k-1}{n} + 2(\lceil \bar{\delta}_+ \rceil - \bar{\delta}_+) & h + \frac{2}{n} < \bar{\delta}_+ < h+1, \\ -4\frac{k-1}{n} + 2 - \frac{4}{n} & \bar{\delta} \leq h. \end{cases}$$

Furthermore, for fixed $n \geq 2$ a number of edges $\underline{m}$ maximizing $\underline{TE}(n,m)$ is $\underline{m} = \underline{k}(\underline{k}+1)/2 + \underline{k}(n-1-\underline{k})$ with $\underline{k} = \lceil \frac{n}{3} \rceil$.

Proof The case distinction is correct, because we cannot have $\bar{\delta}_+ = \bar{\delta} + \frac{2}{n} \leq h + \frac{2}{n} < \bar{\delta}_+$ and once $\bar{\delta} \leq h$ we also have $\bar{\delta} + \frac{2}{n} < h+1$. For $m \geq \frac{n}{2}$ satisfying $\underline{m}_k \leq m \leq \underline{m}_{k+1} - 1$ we have $\underline{f}(n,m) = k$, so $h = k+1+m-\underline{m}_k$ is equal to $\underline{d}^*_{\underline{f}(n,m)}$ in (2), therefore

$$\underline{TE}(n,m) = 2[(k-1)(n-\tfrac{2m}{n}) + \max\{0, h - \tfrac{2m}{n}\}].$$

As the case $h + \frac{2}{n} < \bar{\delta}_+ < h+1$ implies $h+1 = \lceil \bar{\delta}_+ \rceil$, the differences due to adding a single edge are obtained by direct computation.

We proceed to show that for fixed n the maximum value of $\underline{TE}$ must be attained for some k with m at the upper boundary. For $k \in [n-2]$ the relation $h + \frac{2}{n} < \bar{\delta}_+ < h+1$ implies $\lceil \bar{\delta}_+ \rceil - \bar{\delta}_+ < 1 - \frac{2}{n}$, which ensures $-4\frac{k-1}{n} \leq -4\frac{k-1}{n} + 2(\lceil \bar{\delta}_+ \rceil - \bar{\delta}_+) \leq -4\frac{k-1}{n} + 2 - \frac{4}{n}$. Therefore for each $k \geq 2$ the maxima or obtained at the boundary, thus either for $\underline{m}_k$ or for $\underline{m}_{k+1} - 1$. For $k = 1$ one checks directly that the value grows from $m = 1$ to $m = n-1$ throughout. Stepping to the next $k > 1$, compare $\underline{TE}(n, \underline{m}_k - 1) = 2[(k-2)(n - \frac{2(\underline{m}_k - 1)}{n}) + n - \frac{2(\underline{m}_k - 1)}{n}]$ to $\underline{TE}(n, \underline{m}_k) = 2[(k-1)(n - \frac{2\underline{m}_k}{n}) + \max\{0, k+1-\frac{2\underline{m}_k}{n}\}]$. The value increases only if $k+1 \geq \frac{2\underline{m}_k}{n} + (k-1)\frac{2}{n}$, which simplifies to the condition $k(n+4) \leq 3n$. Hence, the only case with $\underline{TE}(n, \underline{m}_k) > \underline{TE}(n, \underline{m}_k - 1)$ is $k = 2$. For $k = 2$ and $m = \underline{m}_2 = n$ we also have $h = 3 \geq \bar{\delta} = 2$ resulting in $\underline{TE}(n, m'+1) = \underline{TE}(n, m') + 2 - \frac{8}{n}$ for $\underline{m}_2 \leq m' < \underline{m}_3 - 1$, which also holds for $n = 3$ because then $\underline{m}_2 = \underline{m}_3 - 1$. Thus, for fixed n the maximum value of $\underline{TE}$ must be attained for some $\underline{m}_{k+1} - 1$, $k \in [n-1]$.

In order to find the maximizing $k \in [n-1]$, observe that

$$\tfrac{n}{2}\underline{TE}(n, \underline{m}_{k+1} - 1) = k^3 + (1-2n)k^2 + n^2 k. \tag{4}$$

For $k \geq 2$ the difference to the predecessor is $\frac{n}{2}(\underline{TE}(n, \underline{m}_{k+1} - 1) - \underline{TE}(n, \underline{m}_k - 1)) = 3k^2 - (4n+1)k + (n^2 + 2n)$ which is strictly positive for $k < \frac{2}{3}n + \frac{1}{6} - \sqrt{(\frac{n}{3} - \frac{2}{3})^2 - \frac{5}{12}}$. Due to the integrality of k we may ignore the term $-\frac{5}{12}$ below the square root whenever $x - \sqrt{x^2 - \frac{5}{12}} \leq \frac{1}{6}$ which yields the condition $\frac{4}{3} \leq x = \frac{n}{3} - \frac{2}{3}$. Thus for $n \geq 6$ a best k is $k^* = \lfloor \frac{n}{3} + \frac{5}{6} \rfloor = \lceil \frac{n}{3} \rceil$. For $n \in \{2,3,4,5\}$ the same formula holds, as can be verified directly. □

In studying the development of $\overline{TE}(n,m)$ for increasing m the same strategy works out when proceeding in lexicographically minimal order by filling up the elements on and above the diagonal in column-wise order. As before, h holds the row index of the last element in column k, but this time $h < k$ refers to the part above the diagonal. It turns out that the formula for the next column can be continued directly from the diagonal element on the previous column, allowing for a smooth transition between columns in the recurrence relation for $\overline{TE}(n,m)$.

Lemma 4 *Given $n \geq 3$ and m with $k(k+1)/2 \leq m < (k+1)(k+2)/2$ for some $k \in [n-2]$. Put $\bar{\delta}_+ = 2(m+1)/n = \bar{\delta} + \frac{2}{n}$ and $h = m - k(k+1)/2$, then*

$$\overline{TE}(n, m+1) = \overline{TE}(n,m) + \begin{cases} 2 - 4\frac{k}{n} & h+1 \leq \bar{\delta}_+ \\ 4 - 4\frac{k+1}{n} - 2(\bar{\delta} - \lfloor \bar{\delta} \rfloor) & h + \frac{2}{n} < \bar{\delta}_+ < h+1 \\ 4 - 4\frac{k+1}{n} & \bar{\delta} \leq h \end{cases}$$

Furthermore, for fixed $n \geq 3$ a number of edges $\bar{m}$ maximizing $\overline{TE}(n,m)$ is $\bar{m} = \bar{k}(\bar{k}+1)/2$ with $\bar{k} = \lfloor \frac{1}{3}(2n+1) \rfloor$.

Proof The case distinction is correct, because we cannot have $\bar{\delta}_+ = \bar{\delta} + \frac{2}{n} \leq h + \frac{2}{n} < \bar{\delta}_+$ and once $\bar{\delta} \leq h$ we also have $\bar{\delta} + \frac{2}{n} < h+1$. Note that for $k(k+1)/2 \leq m < (k+1)(k+2)/2$ we have $\bar{f}(m) = k$. In contrast, $m = (k+1)(k+2)/2$ yields $\bar{f}(m) = k+1$. Yet, by (3), for all $k(k+1)/2 \leq m \leq (k+1)(k+2)/2$ there holds

$$\overline{TE}(n,m) = 2[(n-(k+1))\tfrac{2m}{n} + \max\{0, \tfrac{2m}{n} - (m - k(k+1)/2)\}].$$

Indeed, for the special case $m = (k+1)(k+2)/2$ we get $m - k(k+1)/2 \geq \frac{2m}{n}$ as well as $\bar{d}^*_{\bar{f}+1} = 0$, so $\overline{TE}(n,m) = 2[(n-1-(k+1))\bar{\delta} + \bar{\delta}]$. The case distinction now discerns which of the terms within the max-expression is active for m and $m+1$. In particular, in the case $h + \frac{2}{n} < \bar{\delta}_+ < h+1$ we use $h = \lfloor \bar{\delta} \rfloor$ in $\max\{0, \bar{\delta} - h\}$. The differences in value due to the additional edge are now obtained by direct computation.

Next, we show that for fixed $n \geq 3$ the number of edges m^* maximizing $\overline{TE}(n,m)$ must satisfy $m^* \in \{k(k+1)/2 \colon k \in [n-1]\}$. This follows once we prove $2 - 4\frac{k}{n} \leq 4 - 4\frac{k+1}{n} - 2(\bar{\delta} - \lfloor \bar{\delta} \rfloor) \leq 4 - 4\frac{k+1}{n}$, because then the maximum will be attained at the boundary. But the condition $h = \lfloor \bar{\delta} \rfloor < \bar{\delta} < \bar{\delta} + \frac{2}{n} = \bar{\delta}_+ < h+1$ shows that $\bar{\delta} - \lfloor \bar{\delta} \rfloor < 1 - \frac{2}{n}$, so the relations hold.

In order to find the maximizing $k \in [n-1]$, observe that

$$\tfrac{n}{2}\overline{TE}(n, k(k+1)/2) = (n-k)k(k+1). \tag{5}$$

Because $\frac{n}{2}(\overline{TE}(n,k(k+1)/2) - \overline{TE}(n,(k-1)k/2)) = (2n+1-3k)k \geq 0$ if and only if $k \leq \frac{1}{3}(2n+1)$, the maximum energy is found for $k^* = \lfloor \frac{1}{3}(2n+1) \rfloor$. □

Comparing both maximizers, we arrive at the following result.

Theorem 5 *For given $n \geq 2$ a threshold graph on n nodes maximizing the Laplacian energy is the Type II graph having conjugate degree sequence $d^*_i = k+1$, $i \in [k]$, and $d^*_{k+i} = 0$, $i \in [n-k]$, with trace $k = \lfloor \frac{1}{3}(2n+1) \rfloor$.*

Proof For the given n let $\underline{m}$, $\bar{m}$ and $\underline{k}$, $\bar{k}$ be as defined in lemmas 3 and 4. By these lemmas it suffices to show $\underline{TE}(n,\underline{m}) \leq \overline{TE}(n,\bar{m})$, or equivalently, by (4) and (5)

$$\underline{k}^3 + (1-2n)\underline{k}^2 + n^2\underline{k} \leq (n-\bar{k})\bar{k}(\bar{k}+1). \tag{6}$$

We prove this by discerning three cases:

Case 1: $n = 3h$ with $h \in \mathbb{N}$: Then $\underline{k} = h$ and $\bar{k} = 2h$. The left hand side of (6) evaluates to $4h^3 + h^2$, the right hand side to $4h^3 + 2h^2$, so (6) holds.

Case 2: $n = 3h+1$ with $h \in \mathbb{N}$: Then $\underline{k} = h+1$ and $\bar{k} = 2h+1$. The left hand side now reads $4h^3 + 5h^2 + 2h + 1$, the right hand side $4h^3 + 6h^2 + 2h$ and (6) holds again.

Case 3: $n = 3h-1$ with $h \in \mathbb{N}$: Then $\underline{k} = h$ and $\bar{k} = 2h-1$. We obtain for the left hand side $4h^3 - 3h^2 + h$ and for the right hand side $4h^3 - 2h^2$, proving the theorem. □

We observe that this maximizer is the disconnected threshold graph consisting of a union of a complete graph of size $\lfloor \frac{2n+1}{3} \rfloor + 1$ with $\lfloor \frac{n-2}{3} \rfloor$ isolated vertices.

Example 6 Let $n = 11$ be the number of nodes. The candidate threshold graphs for largest Laplacian energy are the Type I with number of edges $\underline{m} = \underline{k}(\underline{k}+1)/2 + \underline{k}(n-1-\underline{k}) = 34$ as $\underline{k} = \lfloor \frac{n}{3} + \frac{5}{6} \rfloor = 4$ and the Type II with number of edges $m = k(k+1)/2 = 28$, for $k = \lfloor \frac{2*11+1}{3} \rfloor = 7$. The respective Ferrers diagrams of these graphs are in Figure 5.

The Laplacian energy of the Type I graph (on the left hand side of Figure 5) is 38.545, whereas the Type II (right hand side of Figure 5) has Laplacian energy 40.727, which is in accordance with Theorem 5.

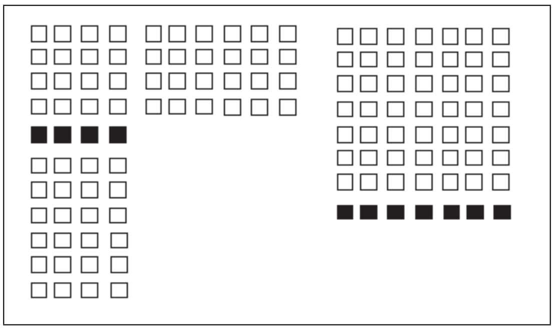

Figure 5: Type I and Type II threshold graph candidates for $n = 11$.

5 Maximal energy for connected threshold graphs

For connected threshold graphs we have $m \geq n - 1$ and $d_1^* = n$. Thus the analysis for the case of Type I with lexicographically maximal conjugate degree sequences can be applied without any changes, and Lemma 3 still determines the best choice of m for given n in the lexicographically maximal setting. The connected Type II case (with lexicographically minimal connected conjugate degree sequence) needs some minor adaptations, but the same line of arguments works out again.

In the connected setting, Lemma 1 reads as follows.

Lemma 7 *Among all connected threshold graphs on n nodes and $m \geq n-1$ edges having a degree sequence with trace f the following are among those with maximal Laplacian energy:*

1. *for $f + 1 \leq \bar{\delta}$ the Type I threshold graph with lexicographically maximal conjugate degree sequence,* i. e. *with $k = \left\lfloor \frac{m-f(f+1)/2}{n-1-f} \right\rfloor$ $(\leq f)$ its first f conjugate degrees are $d_i^* = n$ for $i \in [k]$, $d_i^* = f + 1$ for $i \in \{k+2, \ldots, f\}$ and, if $k < f$, $d_{k+1}^* = f + 1 + m - f(f+1)/2 - k(n-1-f)$,*

2. *for $f + 1 \geq \bar{\delta}$ the connected Type II threshold graph with lexicographically minimal connected conjugate degree sequence,* i. e. *with $h = \left\lfloor \frac{m-n+1-f(f-1)/2}{f-1} \right\rfloor$ and $k = m - n + 1 - f(f-1)/2 - (f-1)h$ $(\leq f)$ its first f conjugate degrees are $d_1^* = n$, $d_i^* = f + h + 2$ for $i \in \{2, \ldots, 1+k\}$ and $d_i^* = f + h + 1$ for $i \in \{k+2, \ldots, f\}$.*

As the proof follows that of Lemma 1 almost verbatim, it is omitted.

Due to the constraint $d_1^* = n$ the upper bound on f is now determined from $f(f-1) \leq 2(m-n+1)$, thus for $n - 1 \leq m \leq n(n-1)/2$ the former $\bar{f}(m)$ is replaced by

$$\bar{f}_c(m) := \left\lfloor \frac{1}{2} + \sqrt{2(m-n) + \frac{9}{4}} \right\rfloor \geq \bar{\delta} - 1.$$

As before, we will only write $\bar{f}_c$ if the argument m is clear form the context. With this we may now adapt the formulation of Theorem 2.

Theorem 8 *The set of connected threshold graphs on n nodes and $m \geq n-1$ edges with maximal Laplacian Energy contains at least one of these: the Type I threshold graph with lexicographically maximal conjugate degree sequence of trace $\underline{f}$ or the connected Type II threshold graph with lexicographically minimal connected conjugate degree sequence of trace $\bar{f}_c$.*

Again the proof is skipped, because the arguments are identical.

For the connected case there is no change in the formula $\underline{TE}(n,m)$ of the Type I threshold graph and for the connected Type II threshold graph with trace $\bar{f}_c$ and lexicographically minimal connected conjugate degree sequence $\bar{d}^c$, one obtains

$$\overline{TE}_c(n,m) := \mathrm{LE}(\mathrm{Th}^*(\bar{d}^*_c)) = 2[(n-2-\bar{f}_c)(\bar{\delta}-1)+\bar{\delta}+\max\{0,\bar{\delta}-\bar{d}^c_{\bar{f}_c+1}\}]$$

with

$$\bar{d}^c_{\bar{f}_c+1} = m-n+2-\bar{f}(\bar{f}-1)/2.$$

Next, we adapt Lemma 4.

Lemma 9 *Given $n \geq 3$ and m with $n-1+k(k-1)/2 \leq m < n-1+k(k+1)/2$ for some $k \in [n-2]$, put $\bar{\delta}_+ = 2(m+1)/n = \bar{\delta}+\frac{2}{n}$ and $h = m-n+2-k(k-1)/2$, then*

$$\overline{TE}_c(n,m+1) = \overline{TE}_c(n,m) + \begin{cases} 2-4\frac{k}{n} & h+1 \leq \bar{\delta}_+ \\ 4-4\frac{k+1}{n}-2(\bar{\delta}-\lfloor\bar{\delta}\rfloor) & h+\frac{2}{n} < \bar{\delta}_+ < h+1 \\ 4-4\frac{k+1}{n} & \bar{\delta} \leq h \end{cases}.$$

Furthermore, for fixed $n \geq 2$ a number of edges $\bar{m}$ maximizing $\overline{TE}_c(n,m)$ is $\bar{m} = n-1+\bar{k}(\bar{k}-1)/2$ with $\bar{k} = \lfloor\frac{2}{3}n\rfloor$.

Proof The case distinction is correct, because we cannot have $\bar{\delta}_+ = \bar{\delta}+\frac{2}{n} \leq h+\frac{2}{n} < \bar{\delta}_+$ and once $\bar{\delta} \leq h$ we also have $\bar{\delta}+\frac{2}{n} < h+1$. For $n-1+k(k-1)/2 \leq m < n-1+k(k+1)/2$ we have $\bar{f}_c(m) = k$, while $m = n-1+k(k+1)/2$ yields $\bar{f}_c(m) = k+1$. For all $n-1+k(k-1)/2 \leq m \leq n-1+k(k+1)/2$ there holds

$$\overline{TE}_c(n,m) = 2[(n-2-k))(\tfrac{2m}{n}-1)+\tfrac{2m}{n}+\max\{0,\tfrac{2m}{n}-(m-n+2-k(k-1)/2)\}].$$

Indeed, for the special case $m = n-1+k(k+1)/2$ we get $m-n+2-k(k-1)/2 \geq \frac{2m}{n}$ as well as $\bar{d}^c_{\bar{f}_c+1} = 1$, so $\overline{TE}_c(n,m) = 2[(n-2-(k+1))(\bar{\delta}-1)+\bar{\delta}+(\bar{\delta}-1)]$. As before, the cases depend on which of the terms within the max-expression are active for m and $m+1$ and follow by direct computation. The case $h+\frac{2}{n} < \bar{\delta}_+ < h+1$ uses $h = \lfloor\bar{\delta}\rfloor$ in $\max\{0,\bar{\delta}-h\}$.

For fixed $n \geq 3$ the number of edges m^* maximizing $\overline{TE}_c(n,m)$ must satisfy $m^* \in \{n-1+k(k-1)/2 \colon k \in [n-1]\}$, because $2-4\frac{k}{n} \leq 4-4\frac{k+1}{n}-2(\bar{\delta}-\lfloor\bar{\delta}\rfloor) \leq 4-4\frac{k+1}{n}$ implies attainment at the boundary. The latter inequalities hold because $\bar{\delta}-\lfloor\bar{\delta}\rfloor < 1-\frac{2}{n}$ is guaranteed by $h = \lfloor\bar{\delta}\rfloor < \bar{\delta} < \bar{\delta}+\frac{2}{n} = \bar{\delta}_+ < h+1$.

In order to find the maximizing $k \in [n-1]$, observe that

$$\tfrac{n}{2}\overline{TE}_c(n,n-1+k(k-1)/2) = (n-k)(n-2+k(k-1))+n = -k^3+k^2(n+1)+k(2-2n)+n^2-n. \tag{7}$$

The difference in values for $k+1$ and k computes to

$$\tfrac{n}{2}(\overline{TE}_c(n,n-1+k(k+1)/2)-\overline{TE}_c(n,n-1+(k-1)k/2)) = -3k^2+k(2n-1)+2-n,$$

which is strictly positive if and only if $k < \frac{n-\frac{1}{2}}{3}+\frac{\sqrt{(n-2)^2+\frac{9}{4}}}{3}$. More generally, the maximizing parameter for $n \geq 2$ is $\bar{k} = \left\lceil \frac{n-\frac{1}{2}}{3}+\frac{\sqrt{(n-2)^2+\frac{9}{4}}}{3} \right\rceil = \lceil\frac{2n}{3}-\frac{5}{6}\rceil$ where the last equation holds for $n \in \{2,\dots,6\}$ by direct computation and for $n \geq 7$, because then $n-\frac{1}{2}+\sqrt{(n-2)^2+\frac{9}{4}}-2n+\frac{5}{2} < \frac{1}{6}$ and integrality of n establish validity. In fact, $\lceil\frac{2n}{3}-\frac{5}{6}\rceil = \lfloor\frac{2n}{3}\rfloor$ holds for $n = 1,2,3$ and thus for all $n \in \mathbb{N}$, so for given $n \geq 2$ the maximum energy is found for $\bar{k} = \lfloor\frac{2n}{3}\rfloor$. □

This allows to identify the Pineapple $P_{n,f'}$, with trace $f' = \lfloor \frac{2n}{3} \rfloor$, as a maximizer of the Laplacian energy among all connected threshold graphs with a given number of nodes.

Theorem 10 *For given $n \geq 2$ a connected threshold graph on n nodes maximizing the Laplacian energy has conjugate degree sequence $d_1^* = n$, $d_i^* = k+1$ for $i \in \{2, \dots, k\}$, $d_i^* = 1$ for $i \in \{k+1, \dots, n-1\}$ and $d_n^* = 0$ with $k = \lfloor \frac{2}{3} n \rfloor$.*

Proof For the given n let $\underline{m}$, $\bar{m}$ and $\underline{k}$, $\bar{k}$ be as defined in lemmas 3 and 9. By these lemmas it suffices to show $\underline{TE}(n, \underline{m}) \leq \overline{TE}_c(n, \bar{m})$, or equivalently, by (4) and (7)

$$\underline{k}^3 + (1 - 2n)\underline{k}^2 + n^2 \underline{k} \leq (n - \bar{k})(n - 2 + \bar{k}(\bar{k} - 1)) + n. \tag{8}$$

Again we prove this by discerning the following three cases:

Case 1: $n = 3h$ with $h \in \mathbb{N}$: Then $\underline{k} = h$ and $\bar{k} = 2h$. The left hand side of (6) evaluates to $4h^3 + h^2$, the right hand side to $4h^3 + h^2 + h$, so (8) holds.

Case 2: $n = 3h + 1$ with $h \in \mathbb{N}$: Then $\underline{k} = h + 1$ and $\bar{k} = 2h$. The left hand side now reads $4h^3 + 5h^2 + 2h + 1$, the right hand side $4h^3 + 5h^2 + 3h$ and (8) holds again.

Case 3: $n = 3h - 1$ with $h \in \mathbb{N}$: Then $\underline{k} = h$ and $\bar{k} = 2h - 1$. We obtain for the left hand side $4h^3 - 3h^2 + h$ and for the right hand side $4h^3 - 3h^2 + 2h - 1$, proving the theorem. □

Example 11 For $n = 11$, the Pineapple $P_{11,7}$ has $m = 31$ edges and largest Laplacian energy among all connected threshold graphs with 11 vertices. We notice that $\mathrm{LE}(P_{11,7}) = 39.091 < 40.727 = \mathrm{LE}(G)$, where G is the Type II threshold graph of Example 6. This is one more instance ascertaining the general belief that, fixing n, the maximal Laplacian energy would be attained by a non connected graph.

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