Maximum Laplacian Energy among Threshold Graphs

Christoph Helmberg (TU Chemnitz)
joint work with
Vilmar Trevisan (UFRGS, Porto Alegre, Brasil)

- Laplacian Energy (LE)
- Threshold Graphs
- Ferrers Diagrams
- Maximal LE(TG) for fixed $n$, $m$, $f$
- Maximal LE(TG) for fixed $n$ and $m$
- Maximal LE(TG) for fixed $n$
- The connected case
- Extensions and Open Problems
The Laplacian Energy of a graph

- finite simple undirected Graph $G = (V, E)$, $n$ nodes $V = \{1, \ldots, n\}$, $m$ edges $E \subseteq \{\{i, j\} : i, j \in V, i \neq j\}$

- Laplacian $[L(G)]_{ij} = \begin{cases} \text{deg}(i) & \text{if } i = j \\ -1 & \text{if } ij \in E \\ 0 & \text{otherwise} \end{cases}$

$L = \begin{bmatrix} 2 & -1 & -1 & 0 \\ -1 & 2 & -1 & 0 \\ -1 & -1 & 3 & -1 \\ 0 & 0 & -1 & 1 \end{bmatrix}$
The Laplacian Energy of a graph

- finite simple undirected Graph $G = (V, E)$, $n$ nodes $V = \{1, \ldots, n\}$, $m$ edges $E \subseteq \{\{i, j\} : i, j \in V, i \neq j\}$ [$ij \in E$]

- Laplacian $[L(G)]_{ij} = \begin{cases} \text{deg}(i) & i = j \\ -1 & ij \in E \\ 0 & \text{otherwise} \end{cases}$

- $L(G) = \sum_{ij \in E} E_{ij}$ $E_{ij} = \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$
The Laplacian Energy of a graph

- **finite simple undirected Graph** $G = (V, E)$,
  - $n$ nodes $V = \{1, \ldots, n\}$,
  - $m$ edges $E \subseteq \{\{i, j\} : i, j \in V, i \neq j\}$

- **Laplacian** $[L(G)]_{ij} = \begin{cases} 
\text{deg}(i) & i = j \\
-1 & ij \in E \\
0 & \text{otherwise}
\end{cases}$

- $L(G) = \sum_{ij \in E} E_{ij}$

- $L$ is pos. semidef., eigenvalues $\lambda_1 \geq \cdots \geq \lambda_{n-1} \geq \lambda_n = 0$.

- average degree $\bar{\delta} = 2m/n$, $\sum_{i \in V} \lambda_i = 2m = n\bar{\delta}$

- **Laplacian Energy** $LE(G) = \sum_{i \in V} |\lambda_i - \bar{\delta}|$

Given $n$, which (connected) graphs maximize the Laplacian Energy?
Pineapple Conjecture

On \( n \) nodes a connected graph maximizing the Laplacian energy is the pineapple graph (a clique on \( \{1, \ldots, \lfloor \frac{2n}{3} \rfloor + 1\} \) plus edges \( \{1, i\} : i = \lfloor \frac{2n}{3} \rfloor + 2, \ldots, n \}).

V. Trevisan
Pineapple Conjecture

On $n$ nodes a connected graph maximizing the Laplacian energy is the pineapple graph

(a clique on $\{1, \ldots, \lfloor \frac{2n}{3} \rfloor + 1\}$ plus edges $\{\{1, i\} : i = \lfloor \frac{2n}{3} \rfloor + 2, \ldots, n\}$).

V. Trevisan

We cannot prove this conjecture, but the pineapple is a threshold graph and we can prove it to be a maximizer over all threshold graphs.

For not necessarily connected graphs we are able to exhibit maximizers over all threshold graphs, split graphs, and cographs. We only discuss the threshold case here.
Threshold Graphs \cite{MahadevPeled1995}

first introduced by Chvátal and Hammer for independent sets

$G$ is a threshold graph if it can be constructed from the one-vertex graph by repeatedly adding an isolated vertex or a dominating vertex (\(=\)connected to all previous ones).

expressed via a 0-1 sequence

0 1 1 1 1 0 0 1
Threshold Graphs [MahadevPeled1995]

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$G$ is a **threshold** graph if it can be constructed from the one-vertex graph by repeatedly adding an isolated vertex or a dominating vertex (=connected to all previous ones).

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degree sequence: 7 5 5 5 5 5 1 1
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![Diagram of a threshold graph]

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$$0 1 1 1 1 0 0 1$$

degree sequence: $7 5 5 5 5 5 1 1$

Denote by $d_1 \geq d_2 \geq \cdots \geq d_n$ the nonincreasing degree sequence of $G$, then $f = \max\{j : d_j \geq j\}$ is called its **trace**, and $d_i^* = \max\{j : d_j \geq i\}, i = 1, \ldots, n$ its **dual degree** sequence. A graph is threshold if and only if $d_i^* = d_i + 1$ for $i = 1, \ldots, f$. $\rightarrow Th(d^*)$. 
Ferrers (or Young) diagram

illustrates a degree sequence by rows of boxes,
e.g. for \( d=(7,6,6,5,4,4,3,1) \) \([n = 8, m = 17, \bar{\delta} = 36/8]\)

\[
\begin{array}{cccccccc}
  d_1^* & d_2^* & d_3^* & d_4^* & d_5^* & d_6^* & d_7^* & d_8^* \\
  d_1 & \blackbox{} & \blackbox{} & \blackbox{} & \blackbox{} & \blackbox{} & \blackbox{} & \blackbox{} \\
  d_2 & \blackbox{} & \blackbox{} & \blackbox{} & \blackbox{} & \blackbox{} & \blackbox{} & \blackbox{} \\
  d_3 & \blackbox{} & \blackbox{} & \blackbox{} & \blackbox{} & \blackbox{} & \blackbox{} & \blackbox{} \\
  d_4 & \blackbox{} & \blackbox{} & \blackbox{} & \blackbox{} & \blackbox{} & \blackbox{} & \blackbox{} \\
  d_5 & \blackbox{} & \blackbox{} & \blackbox{} & \blackbox{} & \blackbox{} & \blackbox{} & \blackbox{} \\
  d_6 & \blackbox{} & \blackbox{} & \blackbox{} & \blackbox{} & \blackbox{} & \blackbox{} & \blackbox{} \\
  d_7 & \blackbox{} & \blackbox{} & \blackbox{} & \blackbox{} & \blackbox{} & \blackbox{} & \blackbox{} \\
  d_8 & \blackbox{} & \blackbox{} & \blackbox{} & \blackbox{} & \blackbox{} & \blackbox{} & \blackbox{} \\
\end{array}
\]

trace = number of black boxes \([f = 4]\)

Diagrams of threshold graphs are “symmetric”.

Note: \( d_i^* \leq f \) for \( i > f \),
\( d_i^* \geq f + 1 \) for \( i \leq f \).

!! For threshold graphs \( \lambda_i = d_i^* \), \( i = 1, \ldots, n \) !! \([\text{Merris94}]\)
Laplacian Energy of Threshold Graphs

\[ LE(Th(d^*)) = \sum_{i \in V} |d_i^* - \bar{\delta}| = \sum_{d_i^* > \bar{\delta}} (d_i^* - \bar{\delta}) + \sum_{d_i^* \leq \bar{\delta}} (\bar{\delta} - d_i^*) \]
Laplacian Energy of Threshold Graphs

$$LE(Th(d^*)) = \sum_{i \in V} |d_i^* - \bar{\delta}| = \sum_{d_i^* > \bar{\delta}} (d_i^* - \bar{\delta}) + \sum_{d_i^* \leq \bar{\delta}} (\bar{\delta} - d_i^*)$$

Note, $$\sum_{i \in V} (d_i^* - \bar{\delta}) = 0,$$
Laplacian Energy of Threshold Graphs

\[
LE(Th(d^*)) = \sum_{i \in V} |d_i^* - \bar{\delta}| = \sum_{d_i^* > \bar{\delta}} (d_i^* - \bar{\delta}) + \sum_{d_i^* \leq \bar{\delta}} (\bar{\delta} - d_i^*)
\]

Note, \(\sum_{i \in V} (d_i^* - \bar{\delta}) = 0\), thus \(\sum_{d_i^* > \bar{\delta}} (d_i^* - \bar{\delta}) = \sum_{d_i^* \leq \bar{\delta}} (\bar{\delta} - d_i^*)\)
Laplacian Energy of Threshold Graphs

$$LE(Th(d^*)) = \sum_{i \in V} |d_i^* - \bar{\delta}| = \sum_{d_i^* > \bar{\delta}} (d_i^* - \bar{\delta}) + \sum_{d_i^* \leq \bar{\delta}} (\bar{\delta} - d_i^*)$$

Note, $\sum_{i \in V} (d_i^* - \bar{\delta}) = 0$, thus $\sum_{d_i^* > \bar{\delta}} (d_i^* - \bar{\delta}) = \sum_{d_i^* \leq \bar{\delta}} (\bar{\delta} - d_i^*)$ and

$$LE(Th(d^*)) = 2 \sum_{d_i^* \geq \bar{\delta}} (d_i^* - \bar{\delta}) = 2 \sum_{d_i^* \leq \bar{\delta}} (\bar{\delta} - d_i^*)$$
Increase LE for fixed \( n, m, f \) by shifting boxes.

For fixed \( f \) and \( f \leq \bar{\delta} \leq f + 1 \), all symmetric box arrangements are fine:

- For arbitrary arrangement, \( \bar{\delta} = f \leq \bar{\delta} \leq f + 1 \)
- For lexmin degree, \( \bar{\delta} = f \leq \bar{\delta} \leq f + 1 \)
- For lexmax degree, \( \bar{\delta} = f + 1 \leq \bar{\delta} \leq f + 1 \)
Increase LE for fixed $n, m, f$ by shifting boxes

For fixed $f$ and $f \leq \bar{\delta} \leq f + 1$, all symmetric box arrangements are fine:

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If $\bar{\delta} < f$, lexmin will be an optimal arrangement:

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lexmin degree
Increase LE for fixed \( n, m, f \) by shifting boxes

For fixed \( f \) and \( f \leq \bar{\delta} \leq f + 1 \), all symmetric box arrangements are fine:

If \( \bar{\delta} < f \), lexmin will be an optimal arrangement:

If \( \bar{\delta} > f + 1 \), lexmax will be an optimal arrangement (examples are big).
Lemma

Among all threshold graphs on $n$ nodes and $m$ edges with degree sequence of trace $f$ the maximum LE is attained for

- the one having lexmin degree sequence if $\bar{\delta} \leq f + 1$,
- the one having lexmax degree sequence if $\bar{\delta} \geq f + 1$. 


Maximum LE for Threshold Graphs with fixed $n, m$

For fixed $n$ and $m$, feasible trace value $f$ satisfy

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

resulting in upper and lower bounds on $f$,

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

Example for $n = 7, m = 11$

lexmin for $f = 3$  
lexmax for $f = 2$  
lexmin for $\bar{f} = 4$
Theorem

For given $n$ and $m$ a threshold graph of maximum $LE$ can be found among the graphs $lexmax$ for $f$ and $lexmin$ for $\overline{f}$.
Theorem
For given $n$ and $m$ a threshold graph of maximum LE can be found among the graphs lexmax for $f$ and lexmin for $\bar{f}$.

Proof.
Let $T$ be a threshold graph of maximum LE for $n$ and $m$, let it have trace $f$.

Case $\bar{\delta} \leq f + 1$:

Case $\bar{\delta} > f + 1$: 
Theorem
For given $n$ and $m$ a threshold graph of maximum $LE$ can be found among the graphs $lexmax$ for $f$ and $lexmin$ for $\bar{f}$.

Proof.
Let $T$ be a threshold graph of maximum $LE$ for $n$ and $m$, let it have trace $f$.

Case $\bar{\delta} \leq f + 1$:
Lemma $\Rightarrow$ we may assume $T$ is $lexmin$ for this trace.
If $f = \bar{f}$ we are done.

Case $\bar{\delta} > f + 1$:
Theorem
For given $n$ and $m$ a threshold graph of maximum LE can be found among the graphs lexmax for $f$ and lexmin for $\bar{f}$.

Proof.
Let $T$ be a threshold graph of maximum LE for $n$ and $m$, let it have trace $f$.

Case $\tilde{\delta} \leq f + 1$:
Lemma $\Rightarrow$ we may assume $T$ is lexmin for this trace.
If $f = \tilde{f}$ we are done.
Otherwise we may increase $f$ and LE by shifting a box like in

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lexmin for $f = 3$

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lexmin for $\tilde{f} = 4$

Case $\tilde{\delta} > f + 1$:
**Theorem**

*For given $n$ and $m$ a threshold graph of maximum LE can be found among the graphs lexmax for $f$ and lexmin for $\bar{f}$.***

**Proof.**

Let $T$ be a threshold graph of maximum LE for $n$ and $m$, let it have trace $f$.

Case $\bar{\delta} \leq f + 1$:

Lemma $\Rightarrow$ we may assume $T$ is lexmin for this trace. If $f = \bar{f}$ we are done.

Otherwise we may increase $f$ and LE by shifting a box like in

![Diagram](image)

lexmin for $f = 3$  lexmin for $\bar{f} = 4$

Case $\bar{\delta} > f + 1$: same argument leads to lexmax for $\bar{f}$.  □
LE Formulas of lexmax for $f$ and lexmin for $\bar{f}$

Given $n$ and $m$, the Laplacian Energy of lexmax for $f$ (conj. degs. $d^*$) reads

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

with

$$d^*_f = f + 1 + m - f(f + 1)/2 - (f - 1)(n - 1 - f).$$

and the Laplacian Energy of lexmin for $\bar{f}$ (conj. degs. $\bar{d}^*$) reads

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

with

$$\bar{d}^*_{\bar{f}+1} = m - \bar{f}(\bar{f} + 1)/2.$$
Maximum LE for Threshold Graphs with fixed $n$

Path:

- Study $TE(n, m)$ (lexmax for $f$) for $m = 1, \ldots, \binom{n}{2} \to \text{best } m$.
- Study $\overline{TE}(n, m)$ (lexmin for $\bar{f}$) for $m = 1, \ldots, \binom{n}{2} \to \text{best } \bar{m}$.
- Compare the two.

We illustrate the idea of the proof for $\overline{TE}(n, m)$ (lexmin).
• $\overline{TE}(n, .)$ is “convex” along columns:

the new box kills 1 unit, but adds $\frac{2}{n}$ to $\bar{\delta}$
• $\overline{TE}(n, .)$ is “convex” along columns:

![Diagram]

the new box kills 1 unit, but adds $\frac{2}{n}$ to $\overline{\delta}$
• \( \overline{TE}(n, .) \) is “convex” along columns:

the new box kills 1 unit, but adds \( \frac{2}{n} \) to \( \delta \)
• $TE(n,\cdot)$ is “convex” along columns:

\begin{itemize}
  \item The new box kills 1 unit, but adds $\frac{2}{n}$ to $\bar{\delta}$
\end{itemize}
• $\overline{TE}(n, .)$ is “convex” along columns:

the new box kills part of a unit, but adds $\frac{2}{n}$ to $\delta$
• $\overline{TE}(n, .)$ is “convex” along columns:

\[ \overline{TE}(n, k \cdot \frac{k+1}{2}) = nk \cdot \left(\frac{k+1}{2} - \delta\right) = \frac{(n-k)k}{2} \]

and is maximized for $k = \lfloor \frac{1}{3} (2n+1) \rfloor$.

Similar arguments show that $\overline{TE}(n, .)$ is maximized for $\overline{m} = n - 1 + \overline{k} \cdot (\overline{k} - 1)/2$ with $\overline{k} = \lfloor \frac{2}{3} n \rfloor$.

the new box adds $\frac{2}{n}$ to $\delta$
• $\overline{TE}(n, .)$ is “convex” along columns:

In particular, if adding the first box of a column increases LE, all boxes in this column increase LE.

the new box adds $\frac{2^n}{n}$ to $\bar{\delta}$
• \( \overline{TE}(n, .) \) is “convex” along columns:

\[
\begin{align*}
0 & \quad 1 & \quad 2 & \quad 3 & \quad 4 & \quad 5 & \quad 6 & \quad 7 \\
\hline
\text{the new box adds } \frac{2}{n} \text{ to } \overline{\delta}
\end{align*}
\]

In particular, if adding the first box of a column increases LE, all boxes in this column increase LE.

→ we only need to compare LE for “full rectangles” (cliques).
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• For $m = k(k + 1)/2, \ k = 1, \ldots, n - 1$ the formula simplifies to

$$\frac{n}{2} \overline{TE}(n, k(k + 1)/2) = nk(k + 1 - \overline{\delta}) = (n - k)k(k + 1).$$

and is maximized for $k = \lfloor \frac{1}{3}(2n + 1) \rfloor$. 
• $\overline{TE}(n,.)$ is “convex” along columns:

![Diagram](attachment:image.png)

the new box adds $\frac{2}{n}$ to $\delta$

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Similar arguments show that $\overline{TE}(n, \cdot)$ is maximized for

$\bar{m} = n - 1 + \bar{k}(\bar{k} - 1)/2$ with $\bar{k} = \lfloor \frac{2}{3}n \rfloor$. 
Theorem

For given $n \geq 2$ a threshold graph on $n$ nodes maximizing the Laplacian energy is the lexmin graph having conjugate degree sequence $d_i^* = k + 1$, $i \in [k]$, and $d_{k+i}^* = 0$, $i \in [n - k]$, with trace $k = \lceil \frac{1}{3}(2n + 1) \rceil$. 
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Proof.

Use $\bar{k} = \lceil \frac{2}{3}n \rceil$ and $k = \lfloor \frac{1}{3}(2n+1) \rfloor$, these give rise to $\bar{m}$, $m$.

Showing $TE(n, m) \leq \overline{TE}(n, \bar{m})$ simplifies to proving

$$k^3 + (1 - 2n)k^2 + n^2k \leq (n - \bar{k})\bar{k}(\bar{k} + 1).$$
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Case 1: $n = 3h$ with $h \in \mathbb{N}$  \rightarrow  $k = h$ and $\bar{k} = 2h$,
left = $4h^3 + h^2$ while right = $4h^3 + 2h^2$.

Case 2: $n = 3h + 1$ with $h \in \mathbb{N}$  \rightarrow  $k = h + 1$ and $\bar{k} = 2h + 1$,
left = $4h^3 + 5h^2 + 2h + 1$ while right = $4h^3 + 6h^2 + 2h$.

Case 3: $n = 3h - 1$ with $h \in \mathbb{N}$  \rightarrow  $k = h$ and $\bar{k} = 2h - 1$,
left = $4h^3 - 3h^2 + h$ while right = $4h^3 - 2h^2$.
The connected case

For connectedness the first row of Ferrers diagram must be full (node 1 is connected to all others).
→ lexmax is identical, the arguments for lexmin have to be adapted a bit. The same steps lead directly to

**Theorem**

*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 $i \in \{2, \ldots, k\}$, $d_i^* = 1$ for $i \in \{k + 1, \ldots, n - 1\}$ and $d_n^* = 0$ with $k = \lfloor \frac{2}{3} n \rfloor$.

This is exactly the pineapple.
Further results, connections, and open problems

- We can prove that for $n \geq 2$ the $\left\lfloor \frac{2}{3}n + \frac{4}{3} \right\rfloor$-clique has maximum LE among all split graphs and cographs and, more generally, among all “spectrally threshold dominated graphs”.

$G = (V, E)$ is s.th.d. if for $k = 1, \ldots, n - 1$ there is a threshold graph $T_k$ on $|V|$ nodes and $|E|$ edges so that $\sum_{i=1}^{k} \lambda_i(G) \leq \sum_{i=1}^{k} \lambda_i(T_k)$.
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- The conjecture that all graphs are spectrally threshold dominated is equivalent to the following conjecture of A. E. Brouwer:
  
  for all graphs $\sum_{i=1}^{k} \lambda_i(G) \leq |E| + k(k + 1)/2$ for $k = 1, \ldots, n$. 


Further results, connections, and open problems

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$G = (V, E)$ is s.th.d. if for $k = 1, \ldots, n−1$ there is a threshold graph $T_k$ on $|V|$ nodes and $|E|$ edges so that $\sum_{i=1}^{k} \lambda_i(G) \leq \sum_{i=1}^{k} \lambda_i(T_k)$

• The conjecture that all graphs are spectrally threshold dominated is equivalent to the following conjecture of A. E. Brouwer: for all graphs $\sum_{i=1}^{k} \lambda_i(G) \leq |E| + k(k + 1)/2$ for $k = 1, \ldots, n$.

• Spectral threshold dominance is maybe stronger than needed.
Further results, connections, and open problems

• We can prove that for $n \geq 2$ the $\left\lfloor \frac{2}{3} n + \frac{4}{3} \right\rfloor$-clique has maximum LE among all split graphs and cographs and, more generally, among all “spectrally threshold dominated graphs”.

$G = (V, E)$ is s.th.d. if for $k = 1, \ldots, n-1$ there is a threshold graph $T_k$ on $|V|$ nodes and $|E|$ edges so that $\sum_{i=1}^{k} \lambda_i(G) \leq \sum_{i=1}^{k} \lambda_i(T_k)$

• The conjecture that all graphs are spectrally threshold dominated is equivalent to the following conjecture of A. E. Brouwer:

for all graphs $\sum_{i=1}^{k} \lambda_i(G) \leq |E| + k(k + 1)/2$ for $k = 1, \ldots, n$.

• Spectral threshold dominance is maybe stronger than needed.

• What can be done for the connected case?