Energies of Graphs and Matrices
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Summary

1. Definitions
   - Energy of Graph

2. Laplacian Energy
   - Laplacian Matrices
   - Edge Deletion

3. Maximum energy

4. The Integral Formula
   - Integral Formula for Laplacian Energy
Adjacency Matrix

Let $G$ be a finite, undirected, simple graph with $n$ vertices and $m$ edges. Define the Adjacency matrix of $G$, as follows:

$$A(G)_{i,j} = \begin{cases} 
1 & \text{if } v_i \text{ and } v_j \text{ are adjacent} \\
0 & \text{if } v_i \text{ and } v_j \text{ are not adjacent}
\end{cases}$$

$A(G)$ is a symmetric matrix whose eigenvalues $\lambda_i$ are real and $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. 
Energy of a Graph

- 1978, I. Gutman defined the energy of a graph $E(G)$ to be the sum of the absolute values of the eigenvalues of its adjacency matrix.

- Concept originated in Chemistry

- Hückel molecular orbital method uses $\pi$-electron energy to compute heat of combustion for hydrocarbons.
Generalizations of Graph Energy

Two generalizations of the concept:

- Nikiforov (2007): The energy of a matrix $A$ is the sum of its singular values (singular values = square roots of the eigenvalues of $AA^*$.) For any $A \in \mathcal{M}_{m,n}$ define the energy of $A$, $\mathcal{E}(A)$,

$$\mathcal{E}(A) = \sum_{i=1}^{m} s_i(A).$$

From above, we note that the usual energy of a graph $G$, $E(G) = \mathcal{E}(A(G))$.

- Gutman and others: For a graph $G$ on $n$ vertices with associated matrix $M$, the energy of $G$ is defined as:

$$E_M(G) = \sum_{i=1}^{n} |\mu_i - \bar{\mu}|$$

where $\mu_i$'s are the eigenvalues of $M$, and $\bar{\mu}$ is the average of those eigenvalues.
Definition of the Laplacian Matrix

- Let $n$ be the number of vertices, and $m$ number of edges.
- Laplacian matrix $L(G) = D(G) - A(G)$ where $D(G)$ is the diagonal matrix of $G$ with $D(G)_{ii} = \text{degree of } v_i$, and $A(G)$ is the adjacency matrix.
- Laplacian matrix is *symmetric, positive semidefinite, singular*.
- Laplacian Energy $LE(G) = \sum_{i=1}^{n} |\lambda_i - \frac{2m}{n}|$ where $\lambda_i$ are the eigenvalues of the Laplacian matrix.
Definition of Signless Laplacian Matrix

- Signless Laplacian matrix $L^+(G) = D(G) + A(G)$ where $D(G)$ is the degree matrix of $G$, and $A(G)$ is the adjacency matrix.
- Signless Laplacian Energy $LE^+(G) = \sum_{i=1}^{n} |\lambda_i - \frac{2m}{n}|$ where $\lambda_i$ are the eigenvalues of the signless Laplacian matrix.
Definitions:

- Let \( A = [a_{ij}] \) be the \( n \)-by-\( n \) matrix with real entries.
- \( A \) is said to be *symmetric* if \( A = A^T \).
- Theorem: *Symmetric* matrices with real entries have real eigenvalues.
Preliminaries on Energy of Graphs:

- $\sqrt{2m + n(n - 1)|\text{det}A|^2/n} \leq E(G) \leq \sqrt{2mn}$ □
- Only edges: $2\sqrt{m} \leq E(G) \leq 2m$
- Only vertices: $2\sqrt{n - 1} \leq E(G) \leq \frac{n}{2}(1 + \sqrt{n})$
- Question: What is the maximal adjacency energy of graphs on $n$ vertices and how to construct such graph? (Hard!)
### Finding Energy for Specific Graphs:

Laplacian Energy for complete graph $K_n$

<table>
<thead>
<tr>
<th>Lemma 1</th>
<th>If $A_{n \times n}$ is nonsingular, and if $c$ and $d$ are $n \times 1$ columns, then $\det(A + cd^T) = \det(A)(1 + d^T A^{-1} c)$.</th>
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| Theorem | Let $L$ be the Laplacian matrix of the complete graph $K_n$, then

1. Characteristic polynomial of $L$ is $\det(\lambda I - L) = \lambda(\lambda - n)^{n-1}$
2. Laplacian Energy of $K_n$ is $LE(K_n) = 2(n - 1)$ |
H is an induced subgraph of G if the vertex set of H, $V(H)$, is a subset of $V(G)$ and the edge set of H, $E(H)$ contains all edges in G that connect two vertices in $V(H)$.

$\tilde{H}$ is the union of H and all other vertices of G (as isolated vertices).
**Ky Fan’s Inequality**

\[ \sum_{i=1}^{n} s_i(X) + \sum_{i=1}^{n} s_i(Y) \geq \sum_{i=1}^{n} s_i(X + Y), \]

where \( X, Y \) are \( n \times n \) matrices.

**Theorem 1 [REU’09]**

Let \( H \) be an induced subgraph of a simple graph \( G \). Suppose \( \tilde{H} \) denotes the union of \( H \) and vertices of \( G - H \) (as isolated vertices). Then

\[ \text{LE}(G) - \text{LE}(\tilde{H}) \leq \text{LE}(G - \text{E}(H)) \leq \text{LE}(G) + \text{LE}(\tilde{H}). \]

**Theorem 2 [REU’09]**

the result in *Theorem 1* also occurs for Signless Laplacian energy,

\[ \text{LE}^+(G) - \text{LE}^+(\tilde{H}) \leq \text{LE}^+(G - \text{E}(H)) \leq \text{LE}^+(G) + \text{LE}^+(\tilde{H}). \]
Proof of Theorem 1

Note that

\[ D(G) = D(\tilde{H}) + D(G - E(H)). \]

Since

\[ A(G) = \begin{bmatrix} A(H) & X^T \\ X & A(G - H) \end{bmatrix} \]

where \( X \) corresponds to the edges connecting \( H \) and \( G - H \), we have

\[ A(G) = \begin{bmatrix} A(H) & 0 \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & X^T \\ X & A(G - H) \end{bmatrix} \]

\[ = A(\tilde{H}) + A(G - E(H)). \]

Therefore,

\[ L(G) = D(G) - A(G) = L(\tilde{H}) + L(G - E(H)). \]
Cont. Proof

Since $m = |E(\tilde{H})| + |E(G - E(H))|$, it results that

$$L(G) - \frac{2m}{n} I = \left( L(\tilde{H}) - \frac{2|E(\tilde{H})|}{n} I \right) + \left( L(G - E(H)) - \frac{2|E(G - E(H))|}{n} I \right).$$

Hence, by Ky Fan’s inequality, we have

$$LE(G) \leq LE(\tilde{H}) + LE(G - E(H)) \quad \Box$$
Lemma

Suppose $\tilde{H}$ consists of $K_2$ and $n - 2$ isolated vertices. Then $LE(\tilde{H}) = \frac{4(n-1)}{n}$.

Corollary [REU'09]

$$LE(G) - \frac{4(n-1)}{n} \leq LE(G - \{e\}) \leq LE(G) + \frac{4(n-1)}{n}.$$ 

Proof.

Apply Theorem 1 with $H = K_2$ and $\tilde{H}$ consists of $K_2$ and $(n - 2)$ isolated vertices.
We can do better!

**Theorem 3**

\[
LE(G) \leq LE(\tilde{H}) + LE(G - E(H)) \leq 4m\left(1 - \frac{1}{n}\right)
\]
Hyperenergetic graphs

- **Initial Conjecture** (1978): Among graph with \( n \) vertices, the complete graph \( K_n \) has the maximum adjacency energy (equal to \( 2(n - 1) \)).
- Soon disproved by Chris Godsil.

**Definition**

A graph \( G \) having energy greater than the complete graph on the same number of vertices is called *hyperenergetic*.

- Gutman performed a useful experiment: Start with \( n \)-isolated vertices, add edges one-by-one uniformly at random, until end up with \( K_n \).
- Their main observation is: The expected energy of a random \((n, m)\)–graph first increases, attain a maximum at some \( m \), then decreases.
Fig. 1. The dependence of the average energy $<E>$ of graphs with $n = 30$ vertices on $m =$ number of edges; energies above the horizontal line correspond to hyperenergetic graphs.

**Figure:** average energy vs. edges on $n=30$
Maximum Laplacian Energy

A pineapple $PA_{pq}$ is a graph obtained from the complete graph $K_p$ by attaching $q$ pendant vertices to the same vertex of $K_p$.

Conjecture

The maximum Laplacian energy among graphs on $n$ vertices has a pineapple $PA_{\left\lceil \frac{2n+1}{3} \right\rceil, \left\lfloor \frac{n-1}{3} \right\rfloor}$.
The Coulson Integral (1940)

Coulson Theorem

If $G$ is a graph on $n$ vertices, then

$$E(G) = \frac{1}{\pi} \text{p.v.} \int_{-\infty}^{+\infty} \left[ n - \frac{ix\phi'(ix)}{\phi(ix)} \right] dx.$$ 

where $\phi$ is the characteristic polynomial of $A(G)$.

We have proved similar integral formulas for the Laplacian, Signless Laplacian, and Distance Energies.
Theorem 6[REU’09]

If G is a graph on \( n \) vertices and \( m \) edges, then

\[
\text{LE}(G) = \frac{1}{\pi} \text{p.v.} \int_{-\infty}^{+\infty} \left[ n - \frac{ix\phi'_{L}(ix)}{\phi_{L}(ix)} \right] dx.
\]

where \( \phi_{L} \) is the characteristic polynomial of \( L(G) - \frac{2m}{n} I \).
Conjecture

We can apply this integral formula for proving the following

\[ \text{LE}(P_n) \leq \text{LE}(T_n) \leq \text{LE}(S_n) \]
Bibliography


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