Energy and Laplacian Energy of Graphs

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Laplacian Matrix

- Let $\mathbf{D}(G) = [d_{ij}]$ be the diagonal matrix associated with the graph G, defined by $d_{ii} = \deg(v_i)$ and $d_{ij} = 0$ if $i \neq j$, and $\mathbf{L}(G) = \mathbf{D}(G) - \mathbf{A}(G)$ be its Laplacian matrix.

Laplacian Eigenvalues

- The Laplacian polynomial of G is the characteristic polynomial of its Laplacian matrix, $\psi(G, \lambda) = \det(\lambda \mathbf{I}_n - \mathbf{L}(G))$. Let $\mu_1 \geqslant \mu_2 \geq \ldots \geq \mu_n$ the Laplacian eigenvalues of G, i. e., the roots of $\psi(G, \lambda)$.

Laplacian Eigenvalues

- It is well known that $\mu_n = 0$ and that the multiplicity of 0 equals to the number of (connected) components of G.

Ivan Gutman and Bo Zhou, Laplacian energy of a graph, Lin. Algebra Appl. **414** (2006) 29–37.

- The Laplacian energy of the graph G is a very recently defined graph invariant defined as

$$LE = LE(G) = \sum_{i=1}^{n} \left| \mu_i - \frac{2m}{n} \right|$$

Laplacian Eigenvalues

- $\Sigma\mu_i = 2m$ and $\Sigma\mu_i^2 = 2m + M_1(G)$, where $M_1(G) = \Sigma d_i^2$.

Graph Operations

- The Cartesian product $G \times H$ of graphs G and H has the vertex set $V(G \times H) = V(G) \times V(H)$ and $(a,x)(b,y)$ is an edge of $G \times H$ if $a = b$ and $xy \in E(H)$, or $ab \in E(G)$ and $x = y$.

Join

- The join $S = G + H$ of graphs G and H with disjoint vertex sets $V_1 = V(G)$ and $V_2 = V(H)$ and edge sets $E_1 = E(G)$ and $E_2 = E(H)$ is the graph union $G_1 \cup G_2$ together with all the edges joining V_1 and V_2.

Graph Operations

- If $G = G_1 + \ldots + G_n$ then we denote G by $\sum_{i=1}^{n} G_i$. In the case that $G_1 = G_2 = \ldots = G_n = H$ then and we denote G by nH.

Topological Index

- A topological index Top(G) of a graph G is a numeric quantity related to G. This means that if G and H are isomorphic then Top(G) = Top(H).
- Obviously, |V(G)| and |E(G)| are topological index.

Topological Index

- The Wiener index W was the first non-trivial topological index to be used in chemistry.
- It is defined as the sum of all distances between vertices of the graph under consideration.

- Wiener H (1947) Structural determination of the paraffin boiling points, *J. Amer. Chem. Soc.*, 69, 17–20.

E. Estrada, Characterization of 3D molecular structure, Chem. Phys. Lett., 319(2000), 713-718.

- The Estrada index EE(G) of the graph G is defined as the sum of e^{λ} over all eigenvalues of G. This quantity, introduced by Ernesto Estrada.

Laplacian Estrada index

- The Laplacian Estrada index LEE(G) of the graph G is defined as the sum of e^{μ} over all Laplacian eigenvalues of G. This quantity.

Main Results

Proposition 1. $LE(G) \geq n\,|\psi(2m/n)|^{1/n}$, with equality if and only if G is a disjoint union of an empty graph and n copies of K_2.

Main Results

- Proposition 1 can be somewhat enhanced.

$$LE(G) \geq \sqrt{Zg - 2m\left(\frac{2m}{n} - 1\right) + \left|\psi\left(G, \frac{2m}{n}\right)\right|^{1/n}}$$

Main Results

- **Proposition 2**. $\left|\left[LE(\overline{G}) - 2\frac{\overline{m}}{n}\right] - \left[LE(G) - 2\frac{m}{n}\right]\right| \leq n - 1$
- with equality if and only if G is empty or complete graph with n vertices.

Main Results

- **Proposition 3.** Let G be a d-regular graph with $d \geq 2$ and L(G) be the line graph of G. Then $LE(G) \leq LE(L(G)) \leq LE(G) + 2n(d-2)$.

Main Results

Proposition 4. If $G_1,\ldots,G_k$ are graphs then

$$\frac{LE\left(\prod_{i=1}^{k} G_i\right)}{\left|\prod_{i=1}^{k} G_i\right|} \leq \sum_{i=1}^{k} \frac{LE(G_i)}{|G_i|}$$

with equality if and only if every G_i is an empty graph.

Main Results

Proposition 5. If G_1, G_2, …G_k are graphs with exactly n vertices and m edges then

$$LE(\sum_{i=1}^{k} G_i) = \sum_{i=1}^{k} LE(G_i) + 2(k-1)(n-2m/n).$$

Main Results

- **Corollary 1.** If G is a graph then LE(kG) = kLE(G) + 2(k-1)(n-2m/n).
- **Corollary 2.** $LE(K_n) = 2(n-1)$ and
- $LE(K_{\underbrace{n,n,\ldots,n}_{k\ times}}) = 2n(k-1)$.

Main Results

- **Lemma 1.** Let G be a graph with exactly n vertices. Then $EE(G) \geq n$ with equality if and only if G is empty.
- **Lemma 2.** If G is a k-regular connected graph then

$$EE(L(G)) = e^{k-2}EE(G) + (m - n)e^{-2}.$$

Main Results

- **Proposition 6.** Suppose G and H are r- and s-regular graphs with exactly p and q vertices, respectively. Then $EE(G + H) = EE(G) + EE(H) - (e^r + e^s) + 2e^{(p+q)/2}Ch(1/2[(r+s)^2+4pq]^{1/2})$.

Main Results

- **Corollary 1.** If G is r-regular n-vertex graph then $EE(2G) = 2EE(G) - 2e^r + 2e$^rCh(n)).
- **Corollary 2.** Let $K_{m,n}$ denote the complete bipartite graph. Then $EE(K_{m,n}) = m + n - 2 + 2Ch(\sqrt{(mn)})$.

Main Results

- **Corollary 3.** If G is r-regular then $EE(3G) = 3EE(G) - 3e^{r} + 2e^{r}Ch(n) + 2e^{2r+2}Ch((3n)/2) - e^{r+n}$.
- **Corollary 4.** $EE(S_{n+1}) = n - 1 + 2Ch(\sqrt{n})$.

Main Results

- **Corollary 5.** $EE(W_{n+1}) = EE(C_n) - e^2 +$
- $2eCh(\sqrt{(n+1)})$.

Main Results

- **Proposition 7.** Suppose G is a r-regular graph. Then

$$EE(\overline{G}) = e^{-1}\sum_{i=1}^{n} e^{-\lambda_i} + e^{n-r+1} - e^{-r-1}$$

- In particular, if G is bipartite then

$$EE(\overline{G}) = e^{-1}EE(G) + e^{n-r+1} - e^{-r-1}$$

Main Results

- Let R(G) be the graph obtained from G by adding a new vertex corresponding to each edge of G and by joining each new vertex to the end points of the edge responding to it.
- **Proposition 8.** $EE(R(C_n)) \leq n(1+e^{1-\sqrt{2}})$.

Main Results

- **Proposition 9.** Suppose $G_1, G_2, \ldots, G_r$ are graphs. Then

$$EE\left(\prod_{i=1}^{r} G_i\right) = \prod_{i=1}^{r} EE(G_i).$$

- In particular, $EE(G^n) = EE(G)^n$.

Main Results

- **Corollary 1.** Let Q_n be a hypercube by 2^n vertices then $EE(Q_n)=EE(K_2{}^n)=2Ch(1)^n$.
- **Corollary 2.** Let R and S be C_4 nanotube and nanotorus, respectively. Then $EE(R) \approx mnI_0{}^2$ and $EE(S) \approx m(n+1)I_0{}^2 - mCosh(2)I_0$.

Laplacian Estrada Index

$$LEE(G) = \sum_{i=1}^{n} e^{\mu_i - \frac{2m}{n}}, 1 \leq i \leq n.$$

Main Results

Proposition 5. The following properties of $L-$Estrada index are hold:

a) $LEE(G) \geq n$ with equality if and only if $G = \bar{K}_n$,

b) Suppose G_1 and G_2 are graphs with $|V(G_i)| = n_i$ and $|E(G_i)| = m_i, i = 1, 2$. Then $LEE(G_1 + G_2) = e^{\frac{2(m_1 n_2 - m_2 n_1) + (n_1 n_2^2 - n_1^2 n_2)}{n_1(n_1+n_2)}} LEE(G_1) + e^{\frac{2(m_2 n_1 - m_1 n_2) + (n_2 n_1^2 - n_2^2 n_1)}{n_2(n_1+n_2)}} LEE(G_2) + e^{\frac{-2(m_1 + m_2 + n_1 n_2)}{n_1+n_2}} (e^{n_1+n_2} - e_1^n - e_2^n + 1)$.

c) $LEE(\prod_{i=1}^{n} G_i) = \prod_{i=1}^{n} LEE(G_i)$. In particular, $LEE(G^n) = LEE(G)^n$.

d) If G is a $r-$regular bipartite graph then $LEE(G) = EE(G)$.

Main Results

- Let G be an (n, m)-graph. Then the Estrada index of G is bounded as:

$$e^{-\frac{2m}{n}}\sqrt{n(n-1)e^{\frac{4m}{n}}+n+8m+2Zg(G)} \leq LEE(G) \leq (n-1+e^{2m})e^{-\frac{2m}{n}}.$$

- Equality on both sides of above inequality is attained if and only if G $\cong$ K_n.

Main Results

- **Corollary.** If G is an r-regular bipartite graph then $(n^2 + 2nr)^{1/2} \leq LEE(G) \leq n - 2 + 2\cosh((nr)^{1/2})$.

Main Results

- If G is an r-regular graph with n vertices then

$$
\begin{aligned}
1+\sqrt{n-2+2nr+4r-4r^2+e^{-2r}+(n-1)(n-2)e^{\frac{2r}{n-1}}} &\leq LEE(G) \\
&\leq n-1-r^2+\frac{nr}{2}+e^{r}.
\end{aligned}
$$

QUESTIONS?

THANK YOU FOR YOUR ATTENTION!