Energy of Graphs

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- Let G be a finite, simple, undirected graph with n number of vertices and m number of edges.
- Vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$.
- Edge set $E(G) = \{e_1, e_2, \ldots, e_m\}$.
- Adjacency matrix of G is an $n \times n$ matrix $A(G) = [a_{ij}]$, in which $a_{ij} = 1$ if the vertex v_i is adjacent to the vertex v_j and $a_{ij} = 0$, otherwise.

- Characteristic plynomial of G is $\phi(G:\lambda) = \det(\lambda I - A(G))$.

- Eigenvalues of $A(G)$, denoted by $\lambda_1, \lambda_2, \ldots, \lambda_n$ are called the eigenvalues of G and their collcetion is called the spectrum of G.

- If $\lambda_1, \lambda_2, \ldots, \lambda_k$ are the distinct eigenvalues of G with respective multiplicities $m_1, m_2, \ldots, m_k$, then

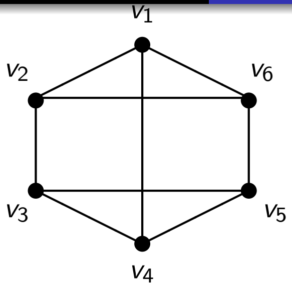
$$Spec(G) = \begin{pmatrix} \lambda_1 & \lambda_2 & \ldots & \lambda_k \\ m_1 & m_2 & \ldots & m_k \end{pmatrix}.$$

Energy of a graph

- The energy of a graph is defined as the sum of the absolute values of the eigenavlues the adjacency matrix of a graph. That is,

$$\mathcal{E}(G) = \sum_{i=1}^{n} |\lambda_i|.$$

- In the matahematical literature, this quantity was putforward in 1978 by Ivan Gutman, but its chemical roots go back to 1930s.



$$\phi(G:\lambda) = \lambda^6 - 9\lambda^4 - 4\lambda^3 + 12\lambda^2$$

$$Spec(G) = \begin{pmatrix} 3 & 1 & 0 & -2 \\ 1 & 1 & 2 & 2 \end{pmatrix}$$

$$\mathcal{E}(G) = 8$$

$$\phi(K_n : \lambda) = (\lambda - n + 1)(\lambda + 1)^{n-1}$$

$$Spec(K_n) = \begin{pmatrix} n-1 & -1 \\ 1 & n-1 \end{pmatrix}$$

$$\mathcal{E}(K_n) = 2(n-1)$$

$$\phi(K_{p,q} : \lambda) = \lambda^{p+q-2}(\lambda^2 - pq)$$

$$Spec(K_{p,q}) = \begin{pmatrix} \sqrt{pq} & 0 & -\sqrt{pq} \\ 1 & p+q-2 & 1 \end{pmatrix}$$

$$\mathcal{E}(K_{p,q}) = 2\sqrt{pq}$$

$$\mathcal{E}(C_n) = \begin{cases} 4\cot\left(\frac{\pi}{n}\right) & \text{if } n \equiv 0 \pmod 4 \\ 4\mathrm{cosec}\left(\frac{\pi}{n}\right) & \text{if } n \equiv 2 \pmod 4 \\ 2\mathrm{cosec}\left(\frac{\pi}{2n}\right) & \text{if } n \equiv 1 \pmod 2 \end{cases}$$

$$\mathcal{E}(P_n) = \begin{cases} 2\mathrm{cosec}\left(\frac{\pi}{2(n+1)}\right) - 2 & \text{if } n \equiv 0 \pmod 2 \\ 2\cot\left(\frac{\pi}{2(n+1)}\right) - 2 & \text{if } n \equiv 1 \pmod 2 \end{cases}$$

One of the remarkable chemical applications of spectral graph theory is based on the close correspondence between the graph eigenvalues and the molecular orbital energy levels of π-electrons in conjugated hydrocarbons.

Hückel Molecular Orbital Theory

- In 1930s, German Scholar Erich Hückel made certain simplification of Schrodinger wave equation.
- The wave functions ψ are the solutions of Schrodinger wave equation $(H - E)\psi = 0$, where H is the energy operator and E is the electron energy.

Hückel replaced the Schrodinger wave function by the secular equation

$$\det(H - ES) = 0$$

where $H = \alpha I + \beta A$ and $S = I + \sigma A$.

Here α (the Coulomb integral for carbon atom), β (the resoannce integral for two carbon atoms) and σ are all constants.

In the ground state, that is when $\alpha = 0$ and $\beta = 1$, H becomes the adjacency matrix $A(G)$ of the associated graph G.

The spectra of graphs can be used to calculate the energy levels of conjugated hydorcarbons as calcultaed with the **Hückel Molecular Orbital method**.

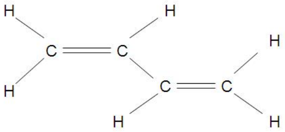


Figure 2: Butadiene C_4H_6 and its molecular graph.

$$H = \begin{bmatrix} \alpha & \beta & 0 & 0 \\ \beta & \alpha & \beta & 0 \\ 0 & \beta & \alpha & \beta \\ 0 & 0 & \beta & \alpha \end{bmatrix} = \alpha I + \beta A$$

As a consequences of above equation, the energy levels ε_i of the π-electrons are related to the eigenvalues λ_i of the graph by the equation

$$\varepsilon_i = \alpha + \beta\lambda_i, \ \ i = 1, 2, \dots n.$$

In the HMO approximation the total energy of the π-electrons is

$$E_\pi = \sum_{i=1}^{n} g_i \varepsilon_i$$

where g_i the count of π-electrons with energy ε_i, called occupation number. Therefore

$$E_\pi = n\alpha + \beta \sum_{i=1}^{n} g_i \lambda_i.$$

The total number of π-electrons is equal to the number of vertices of the associated molecular graph.

For majority of conjugated hydorcarbons, $g_i = 2$ if $\lambda_i > 0$ and $g_i = 0$ if $\lambda_i < 0$. Therfore

$$\begin{aligned} E_\pi &= n\alpha + 2\beta \sum_{+} \lambda_i \\ &= n\alpha + \beta \sum_{i=1}^{n} |\lambda_i|. \end{aligned}$$

Because n, α and β are constants, the only nontrivial term is $\sum_{i=1}^{n} |\lambda_i|$.

Hence the graph energy is [Gutman (1978)]

$$\mathcal{E}(G) = \sum_{i=1}^{n} |\lambda_i|.$$

Coulson integral formula [Coulson (1940)]:

$$\mathcal{E}(G) \;=\; \frac{1}{\pi}\int_{-\infty}^{\infty}\left[n-\frac{\mathbf{i}\lambda\phi'(G:\mathbf{i}\lambda)}{\phi(G:\mathbf{i}\lambda)}\right]d\lambda$$

where $\mathbf{i}=\sqrt{-1}$ and $\phi'(G:\lambda)$ is the first derivative of $\phi(G:\lambda)$.

Proof: Let $\phi(G:\lambda)$ be the polynomial of dgeree n in the complex variable z, and let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be its zeros. Then

$$\phi(G:z) = \prod_{j=1}^{n}(z-\lambda_j)$$

and consequently

$$\frac{\phi'(G:z)}{\phi(G:z)} = \sum_{j=1}^{n}\frac{1}{z-\lambda_j}.$$

Therefore

$$\begin{aligned}
\frac{z\phi'(G:z)}{\phi(G:z)} &= \sum_{j=1}^{n} \frac{z}{z-\lambda_j} \\
&= \sum_{j=1}^{n} \left(1 + \frac{\lambda_j}{z-\lambda_j}\right) \\
&= n + \sum_{j=1}^{n} \frac{\lambda_j}{z-\lambda_j}.
\end{aligned}$$

Therefore

$$\frac{z\phi'(G:z)}{\phi(G:z)} - n = \sum_{j=1}^{n} \frac{\lambda_j}{z-\lambda_j}.$$

And

$$\left[\frac{z\phi'(G:z)}{\phi(G:z)} - n\right] \longrightarrow 0 \quad \text{as} \quad |z| \longrightarrow \infty.$$

Consider the contour Γ^+ shown in the Fig. 4.

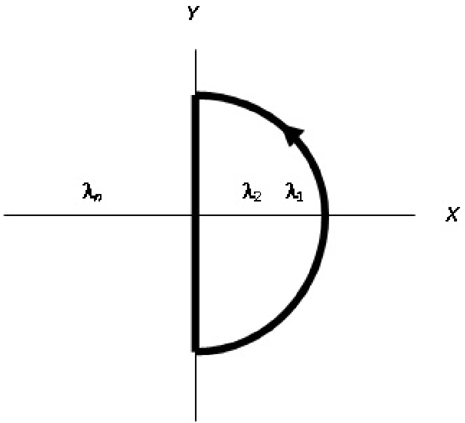


Figure 4: Positively oriented contour Γ^+ in the the complex plane.

According to the well known Cauchy formula

$$\frac{1}{2\pi\mathbf{i}}\oint_{\Gamma^+}\frac{dz}{z-z_0}=\begin{cases}1 & \text{if } z_0\in\operatorname{int}(\Gamma^+)\\ 0 & \text{if } z_0\in\operatorname{ext}(\Gamma^+).\end{cases}$$

Therefore

$$\begin{aligned}\frac{1}{2\pi\mathbf{i}}\oint_{\Gamma^+}\left[\frac{z\phi'(G:z)}{\phi(G:z)}-n\right]dz &= \frac{1}{2\pi\mathbf{i}}\oint_{\Gamma^+}\sum_{j=1}^{n}\frac{\lambda_j}{z-\lambda_j}dz\\ &= \sum_{j=1}^{n}\frac{\lambda_j}{2\pi\mathbf{i}}\oint_{\Gamma^+}\frac{dz}{z-\lambda_j}\\ &= \sum_{+}\lambda_j=\frac{\mathcal{E}(G)}{2}\end{aligned}$$

In the limiting case when Γ^{+} becomes infinitely large, the only non-vanishing contribution to the above integral comes from the intergration along the y-axis.
Thus

$$
\begin{aligned}
\mathcal{E}(G) &= \frac{1}{\pi \mathbf{i}} \oint_{\Gamma^{+}} \left[\frac{z\phi'(G:z)}{\phi(G:z)} - n \right] dz \\
&= \frac{1}{\pi \mathbf{i}} \int_{-\infty}^{\infty} \left[\frac{z\phi'(G:z)}{\phi(G:z)} - n \right] dz + \frac{1}{\pi \mathbf{i}} \int_{\infty}^{-\infty} \left[\frac{z\phi'(G:z)}{\phi(G:z)} - n \right] dz \\
&= 0 + \frac{1}{\pi \mathbf{i}} \int_{\infty}^{-\infty} \left[\frac{\mathbf{i}y\phi'(G:\mathbf{i}y)}{\phi(G:\mathbf{i}y)} - n \right] d(\mathbf{i}y) \\
&= \frac{1}{\pi} \int_{-\infty}^{\infty} \left[n - \frac{\mathbf{i}y\phi'(G:\mathbf{i}y)}{\phi(G:\mathbf{i}y)} \right] dy \\
&= \frac{1}{\pi} \int_{-\infty}^{\infty} \left[n - \frac{\mathbf{i}\lambda\phi'(G:\mathbf{i}\lambda)}{\phi(G:\mathbf{i}\lambda)} \right] d\lambda.
\end{aligned}
$$

Bounds for energy

Theorem (McClelland 1971)

For an (n, m)-graph G,

$$\sqrt{2m + n(n-1)|\det A|^{2/n}} \leq \mathcal{E}(G) \leq \sqrt{2mn}.$$

Proof: Lower bound
Since the GM of positive numbers is not greater than their AM,

$$\begin{aligned}
\frac{1}{n(n-1)} \sum_{i \neq j} |\lambda_i||\lambda_j| &\geq \left(\prod_{i \neq j} |\lambda_i||\lambda_j| \right)^{\frac{1}{n(n-1)}} \\
&= \left(\prod_{i=1}^{n} |\lambda_i|^{2(n-1)} \right)^{\frac{1}{n(n-1)}} \\
&= \left(\prod_{i=1}^{n} |\lambda_i| \right)^{2/n} \\
&= |\det A|^{2/n}.
\end{aligned}$$

Therefore

$$
\begin{aligned}
(\mathcal{E}(G))^2 &= \sum_{i=1}^{n} \lambda_i^2 + \sum_{i \neq j} |\lambda_i||\lambda_j| \\
&\geq 2m + n(n-1)|\det A|^{2/n}.
\end{aligned}
$$

Therefore

$$
\mathcal{E}(G) \geq \sqrt{2m + n(n-1)|\det A|^{2/n}}.
$$

Upper bound
Cauchy-Schawrtz inequality

$$\left(\sum_{i=1}^{n} a_i b_i\right)^2 \leq \left(\sum_{i=1}^{n} a_i^2\right)\left(\sum_{i=1}^{n} b_i^2\right).$$

Let $a_i = 1$ and $b_i = |\lambda_i|$, $i = 1, 2, \ldots, n$.

$$\begin{aligned} \left(\sum_{i=1}^{n} |\lambda_i|\right)^2 &\leq n\sum_{i=1}^{n} |\lambda_i|^2 \\ (\mathcal{E}(G))^2 &\leq n(2m) \\ \mathcal{E}(G) &\leq \sqrt{2mn}. \end{aligned}$$

Equality if and only if $G = (n/2)K_2$.

Theorem (Gutman 2001)

For any graph G with m edges, $2\sqrt{m} \leq \mathcal{E}(G) \leq 2m$.

Proof:

$$
\begin{aligned}
(\mathcal{E}(G))^2 &= \sum_{i=1}^{n} \lambda_i^2 + 2 \sum_{1 \leq i < j \leq n} |\lambda_i||\lambda_j| \\
&\geq 2m + 2 \left| \sum_{i<j} \lambda_i \lambda_j \right| = 2m + 2|-m| = 4m \\
\mathcal{E}(G) &\geq 2\sqrt{m}.
\end{aligned}
$$

For all graphs, $n \leq 2m$.
Therefore $\mathcal{E}(G) \leq \sqrt{2mn} \leq \sqrt{(2m)^2} = 2m$.

Theorem (Koolen, Moulton 2001)

Let G be an (n, m)-graph. If $2m \geq n$, then

$$\mathcal{E}(G) \leq \frac{2m}{n} + \sqrt{(n-1)\left[2m - \left(\frac{2m}{n}\right)^2\right]}.$$

Proof: Cauchy-Schawrtz inequality

$$\left(\sum_{i=1}^{n} a_i b_i\right)^2 \leq \left(\sum_{i=1}^{n} a_i^2\right)\left(\sum_{i=1}^{n} b_i^2\right).$$

Let $a_i = 1$ and $b_i = |\lambda_i|$, $i = 2, 3, \ldots, n$.

$$\begin{aligned}
\left(\sum_{i=2}^{n} |\lambda_i|\right)^2 &\leq (n-1)\sum_{i=2}^{n} |\lambda_i|^2 \\
(\mathcal{E}(G) - \lambda_1)^2 &\leq (n-1)(2m - \lambda_1^2) \\
\mathcal{E}(G) &\leq \lambda_1 + \sqrt{(n-1)(2m - \lambda_1^2).}
\end{aligned}$$

Consider the function $f(x) = x + \sqrt{(n-1)(2m - x^2)}$.

It is decreasing function of the variable $x \in (2m/n, \sqrt{2m})$ and attains at $x = 2m/n$ and $\lambda_1 \geq 2m/n$.

Therefore $f(\lambda_1) \leq f(2m/n)$.

Hence

$$\mathcal{E}(G) \leq \frac{2m}{n} + \sqrt{(n-1)\left[2m - \left(\frac{2m}{n}\right)^2\right]}.$$

Equality holds if and only if $G = (n/2)K_2$ or $G = K_n$ or G is strongly regular graph with two nontrivial eigenvalues both having absolute values equal to

$$\sqrt{\frac{\left[2m - \left(\frac{2m}{n}\right)^2\right]}{(n-1)}}.$$

By immediate consequence of the above inequality it follows that:

Theorem (Koolen, Moulton 2001)

Let G be a graph on n vertices. Then

$$\mathcal{E}(G) \leq \frac{n(\sqrt{n}+1)}{2},$$

with equality if and only if G is strongly regular graph with parameters

$$\left(n, \frac{n+\sqrt{n}}{2}, \frac{n+2\sqrt{n}}{4}, \frac{n+2\sqrt{n}}{4}\right).$$

Above equality holds only for $n = 64, 256, 1024, 4096, \ldots$.

Theorem (Zhou 2004)

If G is a graph with n vertices, m edges and vertex degree sequence $d_1, d_2, \ldots d_n$, then

$$\mathcal{E}(G) \leq \sqrt{\frac{1}{n}\sum_{i=1}^{n} d_i^2 + \sqrt{(n-1)\left[2m - \frac{1}{n}\sum_{i=1}^{n} d_i^2\right]}},$$

with equality if and only if G is either $(n/2)K_2$, K_n, strongly regular graph with two nontrivial eigenvalues both with absolute value $\sqrt{(2m-(2m/n)^2)/(n-1)}$ or nK_1.

Theorem (Zhou and Ramane 2008)

Let G be a bipartite graph with $n \geq 2$ vertices, $m \geq 1$ edges, the first Zagreb index M and an (n_1, n_2)-bipartition, where $n_1 \leq n_2$. If $M \leq \frac{nm}{n_1}$, then

$$\mathcal{E}(G) \leq 2\sqrt{\frac{m}{n_1}} + 2\sqrt{(n_1 - 1)\left(m - \frac{m}{n_1}\right)},$$

with equality if and only if $G = n_1 K_{1,s} \cup (n - n_1 - sn_1)K_1$.

Theorem (Zhou and Ramane 2008)

Let G be a bipartite graph with $n \geq 2$ vertices, $m \geq 1$ edges,and an (n_1, n_2)-bipartition, where $n_1 \leq n_2$. If $m \geq n_2$, then

$$\mathcal{E}(G) \leq \frac{2m}{\sqrt{n_1 n_2}} + 2\sqrt{(n_1 - 1)\left(m - \frac{m^2}{n_1 n_2}\right)}.$$

Let $S_n = K_{1,n-1}$ be the star and P_n be the path on n vertices.

$$\mathcal{E}(S_n) \leq \mathcal{E}(T_n) \leq \mathcal{E}(P_n)$$

Among all trees with n vertices, star has minimum energy and path has maximum energy.

Let $T_1(n)$ be obtained by joining a vertex to a terminal vertex of S_{n-1}.
Let $T_2(n)$ be the tree obtained by joining two vertices to a terminal vertex of S_{n-2}.
Let $T_3(n)$ be the tree obtained by joining a vertex of P_2 to a terminal vertex of S_{n-2}.
Let $T_4(n)$ be the tree obtained by joining a middle vertex of P_5 to the terminal vertex of P_{n-5}.

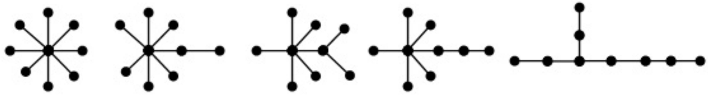


Figure: S_9, $T_1(9)$, $T_2(9)$, $T_3(9)$, $T_4(9)$.

Theorem (Gutman, 1977)
If T is any tree on n vertices different from S_n, $T_1(n)$, $T_2(n)$, $T_3(n)$, $T_4(n)$ and P_n, then

$$\mathcal{E}(S_n) < \mathcal{E}(T_1(n)) < \mathcal{E}(T_2(n)) < \mathcal{E}(T_3(n)) < \mathcal{E}(T) < \mathcal{E}(T_4(n)) < \mathcal{E}(P_n).$$

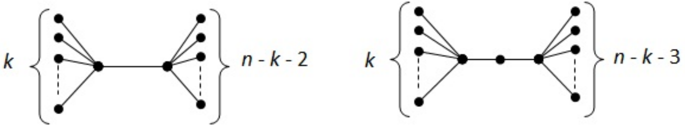


Figure: $A_n(k)$ and $B_n(k)$.

Theorem (Walikar and Ramane 2005)

Let $A_n(k)$ and $B_n(k)$ be the trees as shown above. Then for any two integers n and k,

$$\mathcal{E}(A_n(1)) < \mathcal{E}(A_n(2)) < \cdots < \mathcal{E}(A_n(\lfloor (n/2) - 1 \rfloor))$$

$$\mathcal{E}(B_n(1)) < \mathcal{E}(B_n(2)) < \cdots < \mathcal{E}(B_n(\lfloor (n-3)/2 \rfloor)).$$

Koolen-Moulton (2001) bound is

$$\mathcal{E}(G) \leq \frac{2m}{n} + \sqrt{(n-1)\left[2m - \left(\frac{2m}{n}\right)^2\right]}.$$

If G is an r-regular graph, then

$$\mathcal{E}(G) \leq r + \sqrt{r(n-1)(n-r)}.$$

It is attained for the complete graph.

Let

$$B_2 = r + \sqrt{r(n-1)(n-r)}.$$

Balakrishnan (2004) showed that for $\epsilon > 0$, there exist infinitely many r-regular graphs G such that $\mathcal{E}(G)/B_2 < \epsilon$ and he posed the following problem.

Problem (Balakrishnan 2004)

Given a positive integer $n \geq 3$, does there exist an r-regular graph G of order n, such that $\mathcal{E}(G)/B_2 > 1 - \epsilon$ for some $r < n - 1$?

An affirmative answer to this question is given by Walikar, Ramane, Jog (2008) and by Li, Li, Shi (2010), not for general n but when $n \equiv 1 \pmod 4$, $n \geq 5$.

In both papers same example is considered, namely the Paley graph.

The Paley graph G_p is a strongly regular graph with parameters

$$\left(n, \frac{n-1}{2}, \frac{n-5}{4}, \frac{n-1}{4}\right).$$

It is a regular graph of degree $(n-1)/2$ and

$$Spec(G_p) = \begin{pmatrix} \frac{n-1}{2} & \frac{-1+\sqrt{n}}{2} & \frac{-1-\sqrt{n}}{2} \\ 1 & \frac{n-1}{2} & \frac{n-1}{2} \end{pmatrix}.$$

$$\mathcal{E}(G_p) = \frac{(n-1)(\sqrt{n}+1)}{2}.$$

and

$$\begin{aligned} B_2 &= r + \sqrt{r(n-1)(n-r)} \\ &= \frac{(n-1)(1+\sqrt{n+1})}{2}. \end{aligned}$$

Therefore

$$\frac{\mathcal{E}(G_p)}{B_2} = \frac{\sqrt{n}+1}{1+\sqrt{n+1}} \longrightarrow 1 \text{ as } n \longrightarrow \infty.$$

It follows that for any $\epsilon > 0$ and some integer N, if $n > N$ then

$$\frac{\mathcal{E}(G_p)}{B_2} > 1 - \epsilon.$$

Table: Ratio of $\mathcal{E}(G_p)$ to B_2

n	$\mathcal{E}(G_p) = \frac{(n-1)(\sqrt{n}+1)}{2}$	$B_2 = \frac{(n-1)(1+\sqrt{n+1})}{2}$	$\mathcal{E}(G_p)/B_2$
5	6.472135955	6.8989794856	0.9381294681
101	552.4937811	554.9752469	0.9955286910
525065	190496813.3110102	190496994.46400146	0.9999990490
1011101	508853860.6970579	508854112.1	0.9999995059
102496524	518891553299.8796	518891555830.893789	0.9999999951

Hyperenergetic graphs:

- For molecular graphs McClelland showed that

$$\mathcal{E}(G) \approx a\sqrt{2mn}$$

  where $a \approx 0.9$.

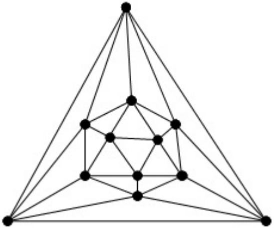
- Among all graphs with n vertices, the complete graph K_n has maximum edges equal to $m = n(n-1)/2$.

- With this observation, Gutman (1978) conjectured that, among all graphs with n vertices, the complete graph has maximum energy.

- That is, if G is any graph with n vertices then

$$\mathcal{E}(G) \leq \mathcal{E}(K_n) = 2(n-1).$$

But this conjecture is not true.



$$Spectra = \begin{pmatrix} 5 & 2.2361 & -2.2361 & -1 \\ 1 & 3 & 3 & 5 \end{pmatrix}$$

$\mathcal{E}(G) \approx 23.4166$ and $\mathcal{E}(K_{12}) = 22$.

- In 1999, Walikar, Ramane and Hampiholi proposed the first systematic construction of infinite number of graphs for which this conjecture does not hold.

- $$Spec(K_n) = \begin{pmatrix} n-1 & -1 \\ 1 & n-1 \end{pmatrix}$$

- $$Spec(L(K_n)) = \begin{pmatrix} 2n-4 & n-4 & -2 \\ 1 & n-1 & n(n-3)/2 \end{pmatrix}$$

- For $n \geq 5$,

$$\mathcal{E}(L(K_n)) = |2n-4|+|n-4|(n-1)+|-2|(n(n-3)/2) = 2n^2-6n$$

- $$\mathcal{E}(K_{n(n-1)/2}) = 2\left(\frac{n(n-1)}{2} - 1\right) = n^2 - n - 2$$

- $\mathcal{E}(L(K_n)) > \mathcal{E}(K_{n(n-1)/2})$.

There are several other examples for which this conjceture does not hold. For instance:

(i) $\overline{L(K_n)}$, $n \geq 6$.

(ii) $L(K_{p,p,})$ and $\overline{L(K_{p,p,})}$, $p \geq 4$.

(iii) A regular graph on $n = 2k$ vertices and of degree $2k - 2$ and its complement, $k > 3$.

A graph G is said to be hyperenergetic if

$$\mathcal{E}(G) > \mathcal{E}(K_n) = 2(n-1)$$

The total graph of G, denoted by $T(G)$ is a graph with vertex set $V(G \cup E(G)$ and two vertices in $T(G)$ are adjacent if and only if the corresponding elements of G are adjacent or incident in G.

Theorem

For any r-regular graph G of order n,
(i) $L(G)$ is hyperenergetic if $r \geq 4$;
(ii) $T(G)$ is hyperenergetic if $r \geq 6$;
where $L(G)$ is the line graph and $T(G)$ is the total graph of G.

Proof:
(i) If $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of a regular graph G, then the eigenvalues of $L(G)$ are $\lambda_i + r - 2$, $i = 1, 2, \ldots, n$ and -2 $(m - n$ times$)$.

$$\begin{aligned} \mathcal{E}(L(G)) &= \sum_{i=1}^{n} |\lambda_i + r - 2| + |-2|(m-n) \\ &\geq \left| \sum_{i=1}^{n} (\lambda_i + r - 2) \right| + 2(m-n) \\ &= n(r-2) + 2(m-n) = 2m + n(r-4) \end{aligned}$$

The graph $L(G)$ is hyperenergetic if $\mathcal{E}(L(G)) > 2(m-1)$.
That is if $2m + n(r-4) > 2m - 2$. It holds if $r \geq 4$.

(ii) If $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of a regular graph G, then the eigenvalues of $T(G)$ are

$$\frac{1}{2}\left(2\lambda_i + r - 2 \pm \sqrt{4\lambda_i + r^2 + 4}\right), \quad i = 1, 2, \ldots, n$$

and -2 ($m - n$ times). Therefore

$$\begin{aligned}\mathcal{E}(T(G)) &= \sum_{i=1}^{n}\left|\frac{1}{2}\left(2\lambda_i + r - 2 \pm \sqrt{4\lambda_i + r^2 + 4}\right)\right| + |-2|(m-n)\\ &\geq \left|\sum_{i=1}^{n}\frac{1}{2}\left(2\lambda_i + r - 2 \pm \sqrt{4\lambda_i + r^2 + 4}\right)\right| + 2(m-n)\\ &= n(r-2) + 2(m-n) = 2m + n(r-4).\end{aligned}$$

The order of $T(G)$ is $m + n$. Therefore $T(G)$ is hyperenergetic if $\mathcal{E}(T(G)) > 2(m + n - 1)$. That is $2m + n(r-4) > 2(m + n - 1)$. It holds as $r \geq 6$.

Theorem (Hou, Gutman 2001)

If $m \geq 2n$ then $L(G)$ is hyperenergetic.

Proof: $\phi(L(G):\lambda) = (\lambda+2)^{m-n}\det[(\lambda+2)I - (D(G)+A(G))]$
If $\mu_1, \mu_2, \ldots, \mu_n$ are the eigenvalues of $D(G)+A(G)$ then eigenvalues of $L(G)$ are -2 ($m-n$ times) and $\mu_i - 2$, $i = 1, 2, \ldots, n$.

$$\begin{aligned}
\mathcal{E}(L(G)) &= |-2|(m-n) + \sum_{i=1}^{n} |\mu_i - 2| \geq 2(m-n) + \sum_{i=1}^{n}(|\mu_i| - 2) \\
&= 2(m-n) + \sum_{i=1}^{n}(\mu_i - 2), \quad \text{since} \;\; \mu_i \geq 0 \\
&= 2(m-n) + 2m - 2n = 4(m-n)
\end{aligned}$$

$L(G)$ is hyperenergetic if $4(m-n) > 2(m-1)$.
That is if $m > 2n-1$ then $\mathcal{E}(L(G)) > 2(m-1)$.

Let v be the vertex of a complete graph K_n, $n \geq 3$ and let e_i, $i = 1, 2, \ldots k$, $1 \leq k \leq n-1$ be its distinct edges, all being incident to v. The graph $Ka_n(k)$ is obtained by deleting e_i, $i = 1, 2, \ldots, k$ from K_n.

For $n \geq 3$ and $0 \leq k \leq n-1$, the eigenvalues of $Ka_n(k)$ are -1 ($n-3$ times) and three roots x_1, x_2, x_3 of the equation $x^3 - (n-3)x^2 - (2n-k-3)x + (k-1)(n-1-k) = 0$, of which two (say x_1 and x_2) are positive and one (say x_3) is negative. Therefore

$$\begin{aligned}\mathcal{E}(Ka_n(k)) &= n - 3 + |x_1| + |x_2| + |x_3| \\ &= n - 3 + x_1 + x_2 - x_3.\end{aligned}$$

Thus $\mathcal{E}(Ka_n(k)) > \mathcal{E}(K_n) = 2(n-1)$ if $x_1 + x_2 - x_3 > n + 1$. This is true for $k = 2, n \geq 10$; $k = 3, n \geq 9$; $k = 4, n \geq 9$; $k = 5, n \geq 10$; $k \geq 6$ and $n \geq k + 4$.
This shows that there are hyperenergetic graphs on n vertices for all $n \geq 9$.

Theorem (Walikar, Gutman, Hampiholi, Ramane 2001)

If $m \leq 2n-2$, then G is non-hyperenergetic.

Proof: Koolen-Moulton bound is

$$\mathcal{E}(G) \leq \frac{2m}{n} + \sqrt{(n-1)\left[2m - \left(\frac{2m}{n}\right)^2\right]}.$$

If

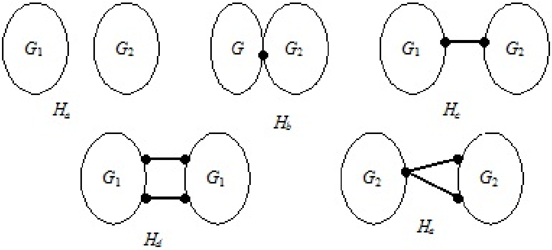
$$\frac{2m}{n} + \sqrt{(n-1)\left[2m - \left(\frac{2m}{n}\right)^2\right]} < 2(n-1)$$

then G is non-hyperenergetic. This equation reduces to

$$[m - 2(n-1)][m - (n(n-1)/2)] > 0.$$

It is true for $m > n(n-1)/2$ and $m < 2(n-1)$. The condition $m > n(n-1)/2$ is impossible. Therefore there remains $m < 2(n-1)$. Hence the proof.

Let G_1 be (n_1, m_1)-graph such that $m_1 \leq 2n_1 - 2$.
Let G_2 be (n_2, m_2)-graph such that $m_2 \leq 2n_2 - 2$.



- All graphs whose average vertex degree is less than 3.5 are nonhyperenergetic.
- No Hückel graph is hyperenergetic.
- All 1, 2, 3 regular graphs are nonhyperenergeic.
- All graphs whose blocks have average degree less than 3.5 are nonhyperenergetic.
- All trees are nonhyperenergetic.
- All graphs in which every edge belongs to atmost one cycle (cactii) are nonhyperenergetic.

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Thank You