Energy of Graphs

A few open problems and some suggestions

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Introduction

Energy of a graph is a concept defined in 1978 and originating from theoretical chemistry.

In short, for an n-vertex graph G with adjacency matrix A having eigenvalues $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$, the energy $E(G)$ is defined as

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

It is related to the total π-electron energy in a molecule represented by a (molecular) graph.

Origins

If we would know some chemistry (I don't):

- Hückel molecular orbital theory (HMO),
- π-electrons and their total energy E_π,
- molecular orbital energy levels E_j,
- the HMO Hamiltonian operator $\grave{\mathbf{H}}$
- molecular orbital occupation numbers g_j
- reasons why things are supposed the way they are

then we might fully appreciate the origin of graph energy.

But, does this matter?

HMO is old

Actually, it does!

In a private communication, Gutman claimed that the HMO theory is nowadays superseeded by new theories that provide better explanations and which do not make unnecessary assumptions.

Limited applications

While HMO has the advantage of being simple and while still used in theoretical chemistry papers, it just won't be used when it comes to investing million$ in synthesizing new molecules.

Thus, the energy of a graph is a mathematical concept that nowadays has LIMITED applications in theoretical chemistry.

The question

Still, it is a challenging mathematical concept!
The leading open problem is:

Which graph on n vertices has the maximum energy?

The rest of the talk is organized as follows:

- Preliminaries
- Trees are Ok
- Bounds
- Hyperenergetic graphs
- Alternative energy definitions

Preliminaries

In the rest of the talk, we suppose:

- G is a simple graph with n vertices and m edges,
- having the adjacency matrix $A = [a_{ij}]$ and
- the eigenvalues $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$.

Two most basic eigenvalue properties are:

- $\sum_i \lambda_i^k =$ the number of closed walks in G of length k;
- *Interlacing*: if $H = G - u$ has eigenvalues $\mu_1 \geq \mu_2 \geq \ldots \geq \mu_{n-1}$, then

$$\lambda_1 \geq \mu_1 \geq \lambda_2 \geq \mu_2 \geq \ldots \geq \lambda_{n-1} \geq \mu_{n-1} \geq \lambda_n.$$

Preliminaries (2)

Special cases that will be needed later are:

$$\sum_i \lambda_i = 0.$$

$$\sum_i \lambda_i^2 = 2m.$$

And, as their consequence,

$$\sum_{i<j} \lambda_i \lambda_j = -m.$$

Energy of subgraphs

From the interlacing property it follows that

$$E(G - u) \leq E(G)$$

for any vertex u. The same inequality extends to any induced subgraph of G.

On the other hand, it is not known under what conditions on the edge e holds that

$$E(G - e) \leq E(G).$$

Coulson Integral Formula

Let $\phi(x)$ be the characteristic polynomial of G,

$$\phi(x) = \det(\lambda I - A) = \sum_{i=0}^{n} a_i x^{n-i}.$$

The Coulson integral formula (1940):

$$E(G) = \frac{1}{\pi} \int_{-\infty}^{\infty} \left(n - x \frac{d}{dx} \log \phi(ix) \right) dx$$

Coulson Integral Formula (2)

Gutman gave alternative representation of the Coulson integral formula

$$E(G) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{dx}{x^2}\ln\left[\left(\sum_{j=0}^{\lceil n/2\rceil}(-1)^j a_{2j}x^{2j}\right)^2 + \left(\sum_{j=0}^{\lceil n/2\rceil}(-1)^j a_{2j+1}x^{2j+1}\right)^2\right].$$

Trees are Ok!

If G is acyclic, its characteristic and matching polynomials are identical,

$$\phi(x) = \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k m_k(G) x^{n-2k},$$

where $m_k(G)$ is the number of matchings of size k.

Further, if T_1 and T_2 satisfy

$$m_k(T_1) \geq m_k(T_2) \quad \text{for all } k = 0, \ldots, \lfloor n/2 \rfloor,$$

then, by the Coulson integral formula,

$$E(T_1) \geq E(T_2).$$

Trees are Ok! (2)

Comparing the trees by their matching numbers,
Gutman was able to show that

$$E(S_n) < E(T) < E(P_n), \qquad T \not\cong S_n, P_n,$$

where S_n is the star and P_n is the path on n vertices.

Quite similarly, one can order bipartite graphs
by the coefficients of their characteristic polynomials
to get corresponding inequality between their energies.

Obtaining max energy trees/simple bipartite graphs is then
a matter of *mastering the characteristic polynomials*,
not an evidence of a deeper knowledge about the energy!

Trees are Ok! (3)

For example, the following special problems have been solved in this way:

- max and min E. for trees with perfect matchings;
- min E. for trees with a given maximum matching size;
- max E. for trees with n vertices and max degree Δ;
- min E. for trees with n vertices and max deg $\Delta \geq \lceil \frac{n+1}{3} \rceil$;
- min E. for trees with n vertices and k pendant vertices;
- min E. for unicyclic graphs;
- max E. for bipartite unicyclic graphs; !!!
- max and min E. for hexagonal chains;
- min E. for chains with polygons of $4n - 2$ vertices.

Conjecture for unicyclic graphs

There exists a conjecture for max E among all unicyclic graphs by Caporossi, Cvetković, Gutman and Hansen.

Let P_n^6 be the unicyclic graph obtained by connecting a vertex of C_6 with a terminal vertex of P_{n-l}.

Conjecture 1 *Among unicyclic graphs on n vertices the circuit C_n has maximum energy if $n \leq 7$ and $n = 9, 10, 11, 13$ and 15. For all other values of n the unicyclic graph with maximum energy is P_n^6.*

Bounds

There is a number of simple (mostly lower) bounds on the energy of graphs.

- McClelland's bounds (1971):

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

Upper bound: Apply the Cauchy-Schwartz inequality to $(1, 1, \ldots, 1)$ and $(|\lambda_1|, |\lambda_2|, \ldots, |\lambda_n|)$ to get

$$E(G) \leq \sqrt{n}\sqrt{\sum_i \lambda_i^2} = \sqrt{n}\sqrt{2m} = \sqrt{2mn}.$$

Bounds (2)

Lower bound: Uses the arithmetic-geometric means inequality

$$E^2(G) = \left(\sum_i |\lambda_i|\right)^2 = \sum_i |\lambda_i|^2 + 2\sum_{i<j} |\lambda_i \lambda_j|$$

$$= 2m + n(n-1)AM(|\lambda_i \lambda_j|) \geq 2m + n(n-1)GM(|\lambda_i \lambda_j|).$$

$$GM(|\lambda_i \lambda_j|) = \left(\prod_{i<j} |\lambda_i \lambda_j\right)^{2/(n^2-n)} = \left(\prod_i |\lambda_i|^{n-1}\right)^{2/(n^2-n)}$$

$$= \left(\prod_i |\lambda_i|\right)^{2/n} = |\det A|^{2/n}.$$

Bounds (3)

Caporossi, Cvetković, Gutman, Hansen (1999):

- $E(G) \geq 2\sqrt{m}$, equality for complete bipartite graphs

$$E^2(G) = 2m+2\sum_{i<j}|\lambda_i\lambda_j| \geq 2m+2\left|\sum_{i<j}\lambda_i\lambda_j\right| = 2m+2|-m| = 4m.$$

- $E(G) \geq \frac{4m}{n}$, equality for complete multipartite graphs

$$\frac{2m}{n} \leq \lambda_1 \leq \sum_{\lambda_i>0}\lambda_i = \frac{1}{2}E(G).$$

Bounds (4)

- Gutman (2001): If G has no isolated vertices, then $E(G) \geq 2\sqrt{n-1}$, with equality for stars.

G is connected: $m \geq n-1$ and $E(G) \geq 2\sqrt{m} \geq 2\sqrt{n-1}$, equality for a complete bipartite graph having $m = n-1$.

G is disconnected with p components:

$$
\begin{aligned}
E(G) &\geq 2\left(\sqrt{n_1 - 1} + \sqrt{n_2 - 1} + \ldots + \sqrt{n_p - 1}\right) \\
&\geq 2\sqrt{n - 1 + (p-1)^2}.
\end{aligned}
$$

In other words: *Among n-vertex graphs without isolated vertices, the star has minimum energy*.

The Koolen-Moulton bounds

The most informative bounds are those of:

- Koolen and Moulton (2001): If G has n vertices, then

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

- Koolen and Moulton (2003): If G has n vertices and it is bipartite, then

$$E(G) \leq \frac{1}{\sqrt{8}} n(\sqrt{n} + \sqrt{2}).$$

They provide *infinite family of maximum energy graphs!*

Strongly regular graphs

A k-regular graph G on n vertices is *strongly regular* with parameters (n, k, λ, μ) if:

- each pair of adjacent vertices has λ common neighbors;
- each pair of non-adjacent vertices has μ common neighbors.

If $\mu = 0$, G is a disjoint union of complete graphs.
If $\mu \geq 1$, the eigenvalues of G are k and the roots r, s of

$$x^2 + (\mu - \lambda)x + (\mu - k) = 0.$$

The eigenvalue k has multiplicity one, whereas the multiplicities m_r of r and m_s of s can be found from

$$m_r + m_s = n - 1, \qquad k + m_r r + m_s s = 0.$$

Edge version of the K-M bound

Theorem 1 (K-M(2001)) *If $2m \geq n$ and G is a graph on n vertices with m edges, then the inequality*

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

holds. Moreover, equality holds if and only if G is either $\frac{n}{2}K_2$, K_n, or a non-complete connected strongly regular graph with two non-trivial eigenvalues both with absolute value $\sqrt{(2m - (\frac{2m}{n})^2)/(n-1)}$.

Proof of the edge K-M bound

First, we have that

$$\sum_{i=2}^{n} \lambda_i^2 = 2m - \lambda_1^2.$$

Applying the Cauchy-Schwartz inequality to the vectors $(1, \ldots, 1)$ and $(|\lambda_2|, \ldots, |\lambda_n|)$ gives

$$\sum_{i=2}^{n} |\lambda_i|^2 \leq \sqrt{(n-1)(2m - \lambda_1^2)}.$$

Hence

$$E(G) \leq \lambda_1 + \sqrt{(n-1)(2m - \lambda_1^2)}.$$

Proof of the edge K-M bound (2)

The function

$$F(x) = x + \sqrt{(n-1)(2m - x^2)}$$

is decreasing on the interval $\sqrt{2m/n} < x \leq \sqrt{2m}$, and since $2m \geq n$,

$$\sqrt{\frac{2m}{n}} \leq \frac{2m}{n} \leq \lambda_1 \leq \sqrt{2m}.$$

Hence, $F(\lambda_1) \leq F(2m/n)$ from which it follows that

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

Equality case in edge K-M bound

From $F(\lambda_1) = F(2m/n)$, it must hold that

$$\lambda_1 = 2m/n.$$

From the Cauchy-Schwartz, it must hold that

$$|\lambda_i| = \sqrt{\frac{2m - \left(\frac{2m}{n}\right)^2}{n-1}}, \qquad 2 \leq i \leq n.$$

Thus, G is regular of degree $2m/n$ and either:

- G has 2 eigenvalues with equal abs. values: $G \cong \frac{n}{2}K_2$,
- G has 2 eigenvalues with distinct abs. values: $G \cong K_n$,
- G has 3 eigenvalues with distinct abs. values: G is a non-complete connected strongly regular graph.

Vertex version of K-M bound

The bound

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

now follows from the previous inequality by noticing that its right hand side—considered as a function of m—is maximized when

$$m = \frac{n^2 + n\sqrt{n}}{4}.$$

Equality holds for a strongly regular graph with parameters $(n, (n + \sqrt{n})/2, (n + 2\sqrt{n})/4, (n + 2\sqrt{n})/4)$.

Infinite family of maximum energy graphs

F. De Clerck and H. Van Maldeghem, *Some classes of rank 2 geometries*, in: Handbook of Incidence Geometry, Elsevier, Amsterdam/New York, 1995.

For each $m \geq 1$, there exists a semipartial geometry with parameters

$$(2^{m+1}-1, 2^{m+2}, 2^m, 2^{m+1}(2^{m+1}-1)).$$

Its point graph is strongly regular with parameters ($\tau = 2^{m+1}$)

$$(4\tau^2, (\tau-1)(2\tau+1), (\tau-2)(\tau+1), \tau(\tau-1)).$$

Its complement is also strongly regular with parameters

$$(4\tau^2, \tau(2\tau+1), \tau(\tau+1), \tau(\tau+1)).$$

What Jack and Vince really hope for?

The last sentence from their 2001 paper is:

Also, for given $\epsilon > 0$ *we suspect that*

for almost all $n \geq 1$
there exists a graph G *on* n *vertices for which*

$$E(G) \geq (1 - \epsilon)\frac{n}{2}(\sqrt{n} + 1).$$

Koolen-Moulton for bipartite graphs

Using exactly the same proof technique and the fact that bipartite graphs have symmetric spectrum, they get:

- energy bound depending on n and m

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

- energy bound depending on n only

$$E(G) \leq \frac{1}{\sqrt{8}} n(\sqrt{n} + \sqrt{2});$$

- cases of equality characterized in both cases;
- an infinite family of maximum energy bipartite graphs.

Hyperenergetic graphs

Initial conjecture (1978):

> Among graphs with n vertices the complete graph K_n has the maximum 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*.

An Energy Experiment

Gutman et al. [a] performed a useful experiment:

> *Start with $\overline{K}_n$, add egdes 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, attains a maximum E_{max} at some $m = m_{max}$ and then decreases.*

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[a] I. Gutman, T. Soldatović, D. Vidović, *The energy of a graph and its size dependence. A Monte Carlo approach*, Chem. Phys. Lett. 297 (1998), 428–432.

Dependence of the average energy [a]

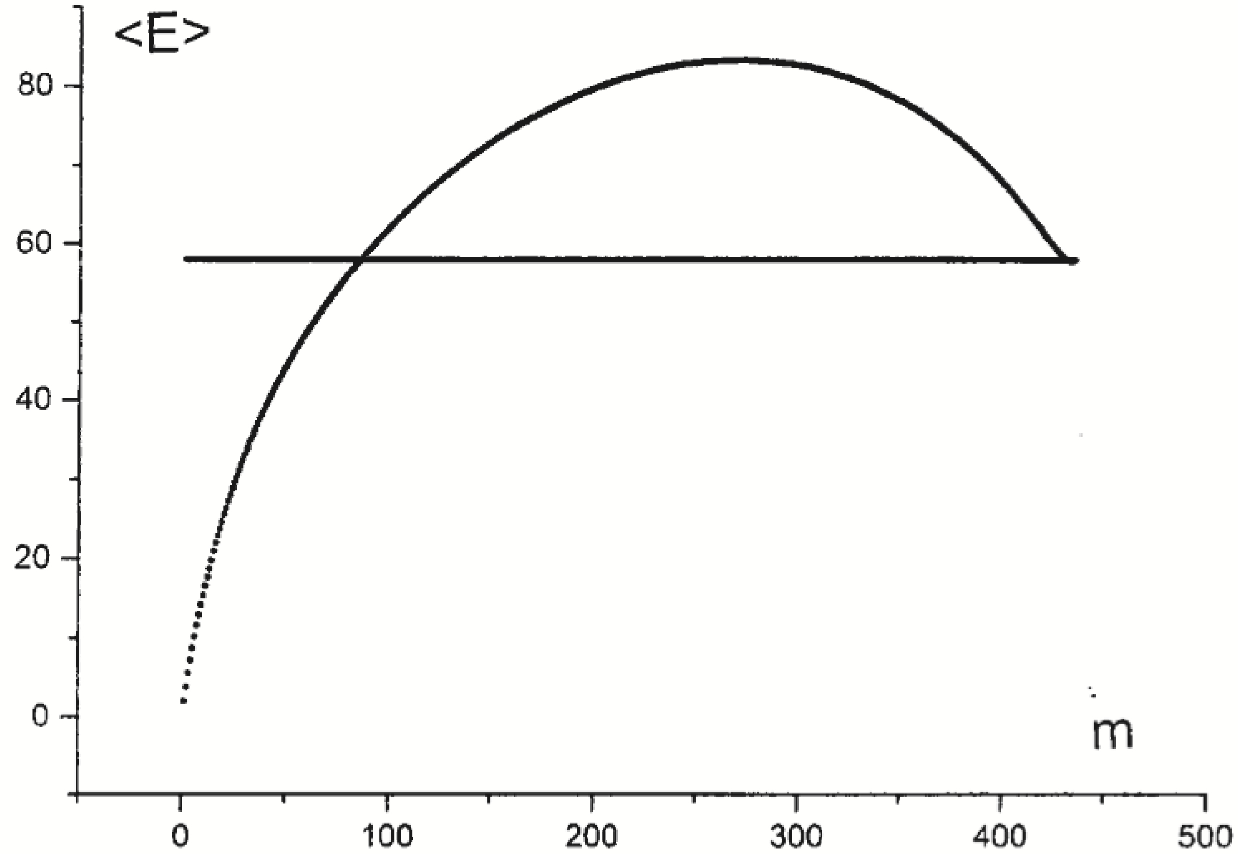

Fig. 1. The dependence of the average energy $<E>$ of graphs with $n = 30$ vertices on m = number of edges; energies above the horizontal line correspond to hyperenergetic graphs.

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[a] Koolen, Moulton, Gutman, Vidović, *More hyperenergetic molecular graphs*, J. Serb. Chem. Soc. 65 (8) (2000), 571–575.

Plenty of graphs are hyperenergetic

They found the following approximate behaviour for $9 \le n \le 30$:

$$\begin{aligned} E_{max} &\approx (0.733 \pm 0.007)\, n^{1.390 \pm 0.004}, \\ m_{max} &\approx (0.47 \pm 0.03)\, n^{1.87 \pm 0.02}. \end{aligned}$$

Compare with K_n:

$$\begin{aligned} E_{K_n} &= (2 - 2/n)\, n, \\ m_{K_n} &= (0.5 - 0.5/n)\, n^2. \end{aligned}$$

Many, many graphs are hyperenergetic!

Hyperenergetic conference graphs

Koolen, Moulton, Gutman, Vidović, *More hyperenergetic molecular graphs*, J. Serb. Chem. Soc. 65 (8) (2000), 571–575.

Conference graph Cf is a strongly regular graph with parameters $(n = 4t+1, 2t, t-1, t)$. It has eigenvalues

$$2t, \qquad -\frac{1}{2}\left(1-\sqrt{4t+1}\right)^{(2t)}, \qquad -\frac{1}{2}\left(1+\sqrt{4t+1}\right)^{(2t)},$$

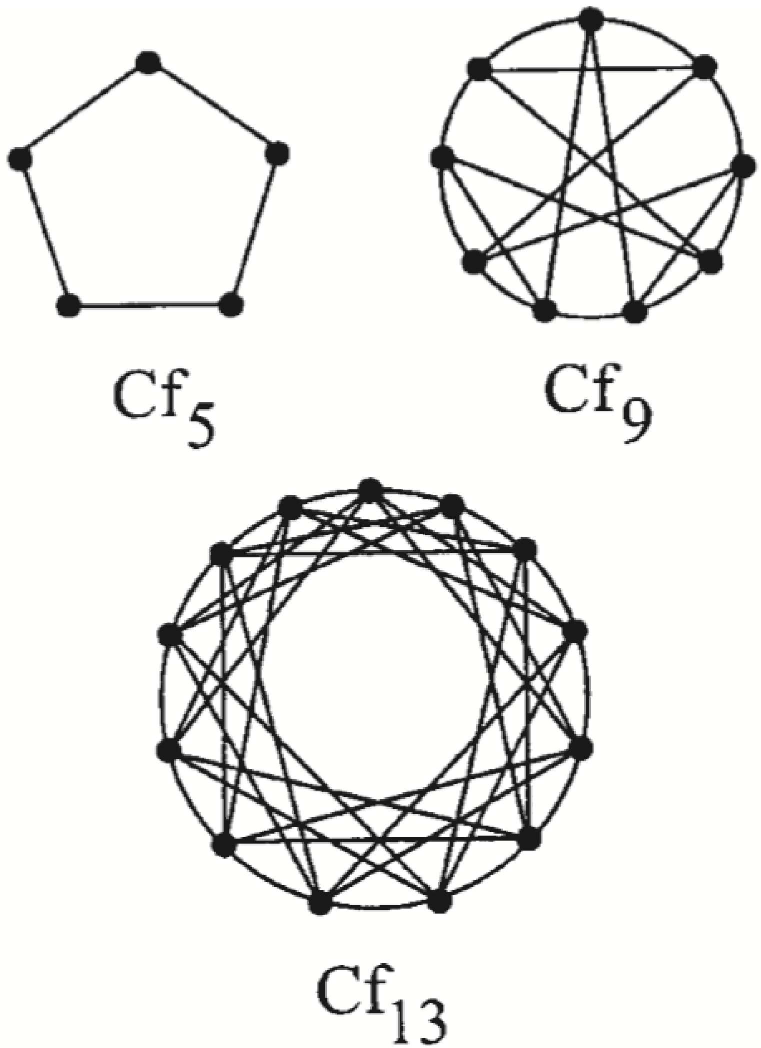
and energy

$$E(Cf) = 2t + 2t\sqrt{4t+1} = \frac{1}{2}(n-1)(\sqrt{n}+1),$$

very close to the Koolen-Moulton bound.

Hyperenergetic conference graphs

There are infinitely many conference graphs, for example, the highly symmetric *Paley graphs*:



Hyperenergetic line graphs

Hou, Gutman, *Hyperenergetic Line Graphs*, Match 43 (2001), 29–39.

Shown that if G has more than $2n-1$ edges,
then its line graph $L(G)$ is necessarily hyperenergetic.

For example, if G is a regular graph of degree r,

$$\phi_{L(G)}(x) = (x+2)^{n(r-2)/2}\phi_G(x-r+2).$$

Eigenvalues of K_n: $n-1$, $-1^{(n-1)}$.
Eigenvalues of $L(K_n)$: $2n-4$, $n-4^{(n-1)}$, $-2^{n(n-3)/2}$.

Energy of $L(K_n)$: $2n^2-6n > n^2-n-2 = E(K_{n(n-1)/2})$.

Hyperenergetic circulant graphs

- Stevanović, Stanković, *Remarks on hyperenergetic circulant graphs*, Linear Algebra Appl. 400 (2005), 345–348.
- Shparlinski, *On the energy of some circulant graphs*, Linear Algebra Appl. 414 (2006), 378–382.

Let $\mathbb{Z}_n$ be the residue ring modulo n, represented by $\{1, \ldots, n\}$.

For $\mathcal{S} \subseteq \{1, \ldots, \lfloor n/2 \rfloor\}$, the *circulant graph* $\mathcal{C}_n(\mathcal{S})$ is a graph whose vertices are elements of $\mathbb{Z}_n$, with the vertex i being adjacent to vertices in $(i - \mathcal{S}) \cup (i + \mathcal{S})$.

Define $\overline{\mathcal{C}}_n(\mathcal{S})$ as the complement of $\mathcal{C}_n(\mathcal{S})$, which is a circulant graph $\mathcal{C}_n(\mathcal{R})$, where $\mathcal{R} = \{1, \ldots, \lfloor n/2 \rfloor\} \setminus \mathcal{S}$.

Hyperenergetic circulants (2)

Start with a FALSE conjecture of Balakrishnan (2004):
$K_n - H$ *is NOT hyperenergetic, for a Hamilton cycle* H.

Note that $K_n - H \cong \overline{\mathcal{C}}_n(\{1\})$.

Let $\mathbf{e}(z) = e^{2\pi\imath z}$, where $\imath = \sqrt{-1}$.
The eigenvalues of $\mathcal{C}_n(\mathcal{S})$ are given by

$$\lambda_j(\mathcal{S}) = \sum_{s \in \mathcal{S} \cup -\mathcal{S}} \mathbf{e}(js/n), \qquad j = 0, 1, \dots, n-1.$$

$$\Rightarrow \qquad \lambda_0(\mathcal{S}) = 2\#\mathcal{S} - \begin{cases} 1, & \text{if } n/2 \in \mathcal{S} \\ 0, & \text{otherwise} \end{cases}$$

Hyperenergetic circulants (3)

$$E(\overline{\mathcal{C}}_n(\{1\})) = n - 3 + \sum_{j=1}^{n-1} \left| -1 - 2\cos\frac{2\pi j}{n} \right|.$$

This is an integral sum:

$$\frac{2\pi}{n-1} \sum_{j=1}^{n-1} \left| -1 - 2\cos\frac{2\pi j}{n} \right| \mapsto \int_0^{2\pi} |-1-2\cos x|\,dx, \qquad n \mapsto \infty.$$

Thus,

$$\lim_{n\mapsto\infty} \frac{E(\overline{\mathcal{C}}_n(\{1\}))}{n-1} = 1 + \frac{1}{2\pi}\int_0^{2\pi} |-1-2\cos x|\,dx = \frac{4\sqrt{3}}{2\pi} + \frac{4}{3} \approx 2.436.$$

Hence, $\mathcal{C}_n(\{1\})$ is hyperenergetic for all $n \geq n_0$ $(= 10)$.

Hyperenergetic circulants (4)

Along the same lines by using the integral sums, one gets

Theorem 2 *For each* $\mathcal{S} = \{k_1, \ldots, k_m\}$*,* $\exists n_0 \in \mathbb{N}$ *such that* $\forall n \geq n_0$*, the graph* $\overline{\mathcal{C}}_n(\mathcal{S})$ *is hyperenergetic.*

This reduces to show that

$$\int_0^{2\pi} \left| -1 - \sum_{i=1}^{m} 2\cos k_i x \right| dx > 2\pi.$$

Hyperenergetic circulants (5)

Since

$$\int_0^{2\pi} \left| -1 - \sum_{i=1}^{m} 2\cos k_i x \right| dx \geq \int_0^{2\pi} 1 + \sum_{i=1}^{m} 2\cos k_i x dx = 2\pi,$$

it remains to show that

$$\max_{x \in [0,2\pi]} -1 - \sum_{i=1}^{m} 2\cos k_i x > 0.$$

Proof of the auxiliary fact

Proof by the Interlacing theorem: for $k = \max \mathcal{S}$ and $n > 4k$, circulant $\overline{\mathcal{C}}_n(\mathcal{S})$ contains P_4 as an induced subgraph (formed by the vertices u, $u+k$, $u+2k$ and $u+3k$).

Thus, the second largest eigenvalue of $\overline{\mathcal{C}}_n(\mathcal{S})$ is at least the second largest eigenvalue of P_4, which is $\frac{-1+\sqrt{5}}{2} \approx 0.618$.

Therefore, for some j_0 it holds that

$$-1 - \sum_{i=1}^{m} 2 \cos k_i \frac{2\pi j_0}{n} \geq \frac{-1+\sqrt{5}}{2}.$$

Hyperenergetic circulants (6)

Shparlinski improved previous theorem to show that

$$\lim_{n\mapsto\infty} \frac{E(\overline{\mathcal{C}}_n(\{s_1,\ldots,s_m\}))}{n} \geq 1+\kappa_{2m},$$

where

$$\kappa_r = \inf_{\#\mathcal{U}=r} \frac{1}{2\pi}\int_0^1 \left|\sum_{u\in\mathcal{U}} \mathbf{e}(\alpha u)\right| d\alpha$$

with the infimum taken over all r-element sets $\mathcal{U}$ of integers. By the Littlewood conjecture:

$$\kappa_r > C\log r$$

for some absolute constant $C>0$ (one may take $C=4/\pi^3$).

Constructions: circulants (7)

Much more important, Shparlinski gave
a construction of high energy circulants.

Let p be a prime number. Denote by $\mathcal{D}_p$ the set of all quadratic residues modulo p in the set $\{1, \ldots, (p-1)/2\}$.

Theorem 3 *For any prime $p \equiv 1 \pmod 4$, we have*

$$E(\mathcal{C}_p(\mathcal{D}_p)) \geq \frac{1}{2}(p-1)(\sqrt{p}+1).$$

This is another type of graphs
that come close to the Koolen-Moulton bound!

Sketch of the proof

-1 is a quadratic residue modulo $p \equiv 1 \pmod 4$
$\Rightarrow \mathcal{D}_p \cup -\mathcal{D}_p$ is the set of all $(p-1)/2$ quadratic residues
$\Rightarrow \#(\mathcal{D}_p \cup -\mathcal{D}_p) = (p-1)/2$
$\Rightarrow \lambda_0(\mathcal{D}_p) = (p-1)/2$

For $j = 1, \ldots, p-1$ we have

$$|\lambda_j(\mathcal{D}_p)| = \sum_{s \in \mathcal{D}_p \cup -\mathcal{D}_p} \mathbf{e}(js/p) = \frac{1}{2} \sum_{u=1}^{p-1} \mathbf{e}(ju^2/p),$$

since for every quadratic residue s
the congruence $s \equiv u^2 \pmod p$ has exactly two solutions.

Sketch of the proof (2)

This is a Gauss sum (Shparlinski says so…):

$$\sum_{u=1}^{p-1} (ju^2/p) = \sum_{u=0}^{p-1} (ju^2/p) - 1 = \begin{cases} \sqrt{p} - 1, & \text{if } j \in \mathcal{D}_p, \\ -\sqrt{p} - 1, & \text{otherwise} \end{cases}$$

Thus,

$$|\lambda_j(\mathcal{D}_p)| = \begin{cases} \frac{1}{2}(\sqrt{p} + 1), & \text{if } j \in \mathcal{D}_p, \\ \frac{1}{2}(\sqrt{p} - 1), & \text{otherwise.} \end{cases}$$

Hence,

$$E(\mathcal{C}_p(\mathcal{D}_p)) \geq \frac{1}{2}(p-1) + (p-1)\frac{\sqrt{p}-1}{2} = \frac{(p-1)(\sqrt{p}+1)}{2}.$$

Expected properties of max-energy graphs

newGRAPH demo: the maximum energy graphs.

Property 1: A maximum energy graph has diameter 2.

(Supported by Gutman's experiment giving the large expected number of edges in such graph.)

Property 2: One large eigenvalue in the spectrum, with the remaining eigenvalues concentrated and more-or-less symmetrically placed in a small interval.

(Supported by the Koolen-Moulton bound.)

Conference graphs and quadratic residue circulants have these properties as well.

Alternative energy definitions

Maximum energy graphs seem to be hard to crack.

On the other hand,
there are other graph spectra in regular use.
Can they yield appropriate energy definitions
that will be easier to study?

Graph related matrices:

- Adjacency matrix A
- Laplacian matrix $L = D - A$
- Signless Laplacian matrix $S = D + A$ (*Dragoš Cvetković*)
- Normalized Laplacian matrix $\tilde{L} = I - D^{-1/2}AD^{-1/2}$ (*Fan Chung*)

How to extend the energy definition?

For A with eigenvalues $\lambda_1^A, \lambda_2^A, \ldots, \lambda_n^A$, the energy is

$$E^A = \sum_{i=1}^{n} \left| \lambda_i^A \right| .$$

For L with eigenvalues $\lambda_1^L, \lambda_2^L, \ldots, \lambda_n^L$, the Laplacian energy is

$$E^L = \sum_{i=1}^{n} \left| \lambda_i^L - \frac{2m}{n} \right| .$$ (*Gutman & Zhou, 2006*)

Note: The average of eigenvalues $\lambda_1^L, \lambda_2^L, \ldots, \lambda_n^L$ is $\frac{2m}{n}$.
The average of eigenvalues $\lambda_1^A, \lambda_2^A, \ldots, \lambda_n^A$ is 0.

Energy of sequences and matrices

Thus, E^A and E^L represent the *absolute deviation from the expected value*.

Definition. The energy E^a of a sequence a: a_1, a_2, ..., a_n with the average value $\bar{a} = \frac{\sum_i a_i}{n}$, is defined by

$$E^a = \sum_{i=1}^{n} |a_i - \bar{a}| \, .$$

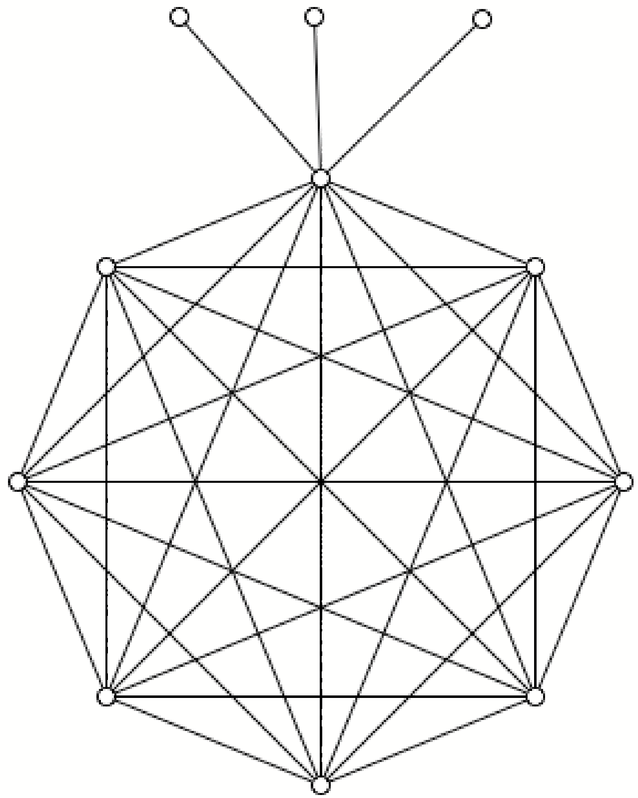
Definition. The energy E^M of a square matrix M is the energy of the sequence of its eigenvalues.

Note that the average of eigenvalues of M is $\frac{trM}{n}$.

Maximum Laplacian energy graphs

Conjecture. The maximum Laplacian energy among graphs on n vertices has a pineaple $PA_{\lceil \frac{2n+1}{3} \rceil, \lfloor \frac{n-1}{3} \rfloor}$.

A *pineaple* $PA_{p,q}$ is a graph obtained from the complete graph K_p by attaching q pendant vertices to the same vertex of K_p.



Maximum Laplacian energy (2)

Pineaple $PA_{p,q}$ appears to have nice Laplacian spectrum:

$$[0, 1^{(q)}, p^{(p-2)}, p+q].$$

(This should be an easy conjecture)

Maximum L.energy is actually obtained for p being the integer closest to

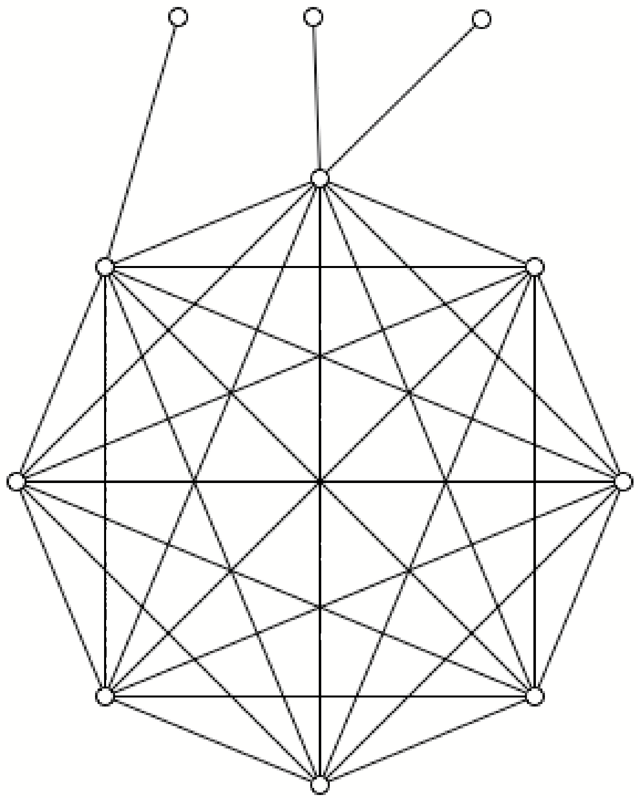
$$\frac{n+4+\sqrt{(n-2)^2+3}}{3}.$$

This seems to always be $\lceil\frac{2n+1}{3}\rceil$.

(Is the latter really true?)

Maximum Laplacian energy (3)

The second maximum L.energy graph is obtained from $PA_{\lceil\frac{2n+1}{3}\rceil,\lfloor\frac{n-1}{3}\rfloor}$ by re-attaching one pendant vertex to another vertex of the complete subgraph.



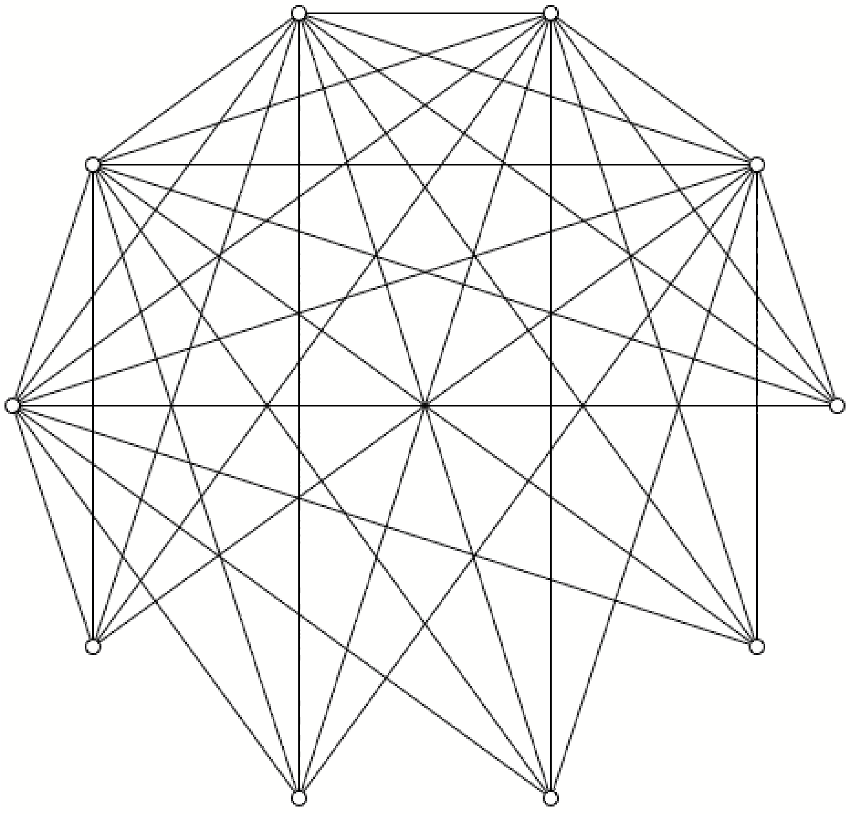
Among the first five L.energy graphs there are *complete split graphs* and *pineaples* with parameters close to optimal values.

newGRAPH demo: maximum L.energy graphs.

Maximum signless Laplacian energy graphs

Conjecture. The maximum signless Laplacian energy among graphs on n vertices has a complete split graph $CS_{\lfloor \frac{n+1}{3} \rfloor, \lceil \frac{2n-1}{3} \rceil}$.

A complete split graph $CS_{p,q}$ is a graph obtained from the complete graph K_p by adding q new vertices each adjacent to each vertex of K_p.



Maximum signless Laplacian energy (2)

Lemma 1 *The signless Laplacian spectrum of $CS_{p,q}$ is:*

$$
\Big[\quad \frac{3p+q-2-\sqrt{(p+q)^2+4(p-1)(q-1)}}{2},
$$

$$
p^{(q-1)},
$$

$$
p+q-2^{(p-1)},
$$

$$
\frac{3p+q-2+\sqrt{(p+q)^2+4(p-1)(q-1)}}{2} \Big].
$$

Proof by straightforward expansion of $|S-\lambda I|$.

Maximum signless Laplacian energy (3)

Among the first five s.L.energy graphs
all graphs are close to complete split graphs.

newGRAPH demo: maximum s.L.energy graphs.

Maximum normalized Laplacian energy

While energy, L.energy and s.L.energy all have
the same order of magnitude,
the normalized Laplacian energy behaves differently:

> *it seems to be maximal for trees, and*
> *it decreases as the edge density increases!*

newGRAPH demo: maximum n.L.energy graphs.

Summary of tasks and problems

1. Which graph on n vertices has maximum energy?
2. Find a better way to apply the Coulson integral formula.
3. Extend the Koolen-Moulton approach to graphs with more than three distinct eigenvalues.
4. Is it true, given $\epsilon > 0$, that for almost all $n \geq 1$ there exists a graph G on n vertices for which
$$E(G) \geq (1-\epsilon)\frac{n}{2}(\sqrt{n}+1)?$$
5. Prove that the pineaple $PA_{\lceil \frac{2n+1}{3} \rceil, \lfloor \frac{n-1}{3} \rfloor}$ has the maximum Laplacian energy.
6. Prove that the complete split graph $CS_{\lfloor \frac{n+1}{3} \rfloor, \lceil \frac{2n-1}{3} \rceil}$ has the maximum signless Laplacian energy.