Energy of a Graph

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Abstract

A discussion of graph energy for the AIM Workshop (October 23–27, 2006): Spectra of Families of Matrices described by Graphs, Digraphs, and Sign Patterns.

1 Graph energy

Let G be a graph (assumed simple throughout) with n vertices and m edges, and let $A = [a_{ij}]$ be the adjacency matrix for G. The eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ of A, assumed in nonincreasing order, are the *eigenvalues of the graph* G. Since A is a symmetric matrix with zero trace, these eigenvalues are real with sum equal to zero. Thus

$$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n, \quad \lambda_1 + \lambda_2 + \cdots + \lambda_n = 0. \tag{1}$$

Considering the coefficient of x^{n-2} in the characteristic polynomial $\phi(x) = \det(xI_n - A)$, we obtain:

$$\sum_{1 \leq i < j \leq n} \lambda_i \lambda_j = -m. \tag{2}$$

We also have

$$2m = \text{trace}(A^2) = \sum_{i=1}^{n} \lambda_i^2. \tag{3}$$

The *energy* of G was first defined by Gutman in 1978 as the sum of the absolute values of its eigenvalues:

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

Since the energy of a graph is not affected by isolated vertices, *we assume throughout that graphs have no isolated vertices implying, in particular, that* $m \geq n/2$. If a graph is not connected its energy is the sum of the energies of its connected components. Thus there is no loss in generality in assuming that graphs are connected, although we don't make this blanket assumption. The concept of graph energy arose in chemistry where certain numerical quantities, such as the heat of formation of a hydrocarbon, are related to total π-electron energy that can be calculated as the energy of an appropriate "molecular" graph (see [4]; where possible, we cite here this survey paper by Gutman in place of specific references). From (1) we obtain

$$\sum\{\lambda_i : \lambda_i > 0\} = -\sum\{\lambda_i : \lambda_i < 0\} = \frac{E(G)}{2}.$$

There is an integral formula for the energy of a graph due to Coulson (1940):

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

where $\phi'(x)$ is its derivative of the characteristic polynomial $\phi(x)$. As a consequence of this formula, a formula is obtained for the difference of the energy of two graphs with the same number of vertices:

$$E(G_1) - E(G_2) = \frac{1}{\pi}\int_{-\infty}^{+\infty}\log\frac{\phi_1(ix)}{\phi_2(ix)}dx.$$

If G is an acyclic graph (so a tree, or a forest if not connected) its characteristic polynomial has the form

$$\phi(x) = x^n + \sum_{k\geq 1}(-1)^k m_k(G)x^{n-2k}$$

where $m_k(G)$ is the number of matchings of G of size k. Making use of this formula, as a corollary of the Coulson integral, Gutman gave a simple formula for the energy of a forest G:

$$E(G) = \frac{1}{\pi}\int_{-\infty}^{+\infty}\frac{dx}{x^2}\log\left(1 + \sum_{k\geq 1}m_k(G)x^{2k}\right).$$

This implies, in particular, that the energy of a forest is a strictly monotonically increasing function of each of the parameters $m_k(G)$. As a consequence one easily gets that, if S_n

and P_n denote, respectively, the *star* and *path* on n vertices, then for every tree T_n on n vertices different from S_n and P_n, we have

$$E(S_n) < E(T_n) < E(P_n).$$

More generally, if G is a bipartite graph with l positive eigenvalues (and so l negative eigenvalues), then

$$\phi(x) = x^n + \sum_{k=1}^{l} (-1)^k b_k(G) x^{n-2k}$$

where $b_k(G) > 0$ for $k = 1, 2, \ldots, l$. In this case we get

$$E(G) = \frac{1}{\pi} \int_{-\infty}^{+\infty} \frac{dx}{x^2} \log \left(1 + \sum_{k \geq 1} b_k(G) x^{2k} \right).$$

Thus the energy of a bipartite graph is a strictly increasing function of each of the parameters $b_k(G)$.

For unicyclic graphs the following conjecture [3] has been made: *Among unicyclic graphs on n vertices, the cycle C_n has the maximal energy if $n \leq 7$ and $n = 9, 10, 11, 13, 15$. For all other values of n, the unicyclic graph P_n^6 obtained by putting a path P_{n-6} at a vertex of a cycle C_6 is the unicycle graph with n vertices of maximal energy.*

As a partial answer to this conjecture, the following has been proved [6]:

Let G be a connected, unicyclic graph whose cycle has even length (G is bipartite) and assume that $G \neq C_n$. Then

$$E(G) < E(P_n^6).$$

2 Energy bounds

Using the arithmetic/geometric mean inequality and the nonnegativity of the variance of nonnegative numbers, McClelland (1971) (for a proof see [4]) gave the following general bounds for energy of a graph with n vertices and m edges with adjacency matrix A (using, in particular, that $\det A = \lambda_1 \lambda_2 \cdots \lambda_n$):

$$\sqrt{2m + n(n-1)|\det A|^{2/n}} \leq E(G) \leq \sqrt{2mn}. \quad (4)$$

The upper bound follows easily using the technique in [7]: Applying the Cauchy-Schwartz inequality to $(1, 1, \ldots, 1)$ and $(|\lambda_1|, |\lambda_2|, \ldots, |\lambda_n|)$, and using (3), we get

$$E(G) \leq \sqrt{n}\sqrt{\sum_{i=1}^{n} \lambda_i^2} = \sqrt{n}\sqrt{2m} = \sqrt{2mn}.$$

Suppose that $\det A \neq 0$. Then G must have at least $n/2$ edges and, since the determinant of the adjacency matrix of a graph is an integer, (4) implies that

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

The energy of a graph as a function of its number n of vertices satisfies:

$$E(G) \leq \sqrt{2mn} \leq \sqrt{2 \cdot n(n-1)/2 \cdot n} = n\sqrt{n-1}. \tag{5}$$

The energy of a graph as a function only of its number of its edges satisfies [3]:

$$2\sqrt{m} \leq E(G) \leq 2m \tag{6}$$

with equality on the left if and only if G is a complete bipartite graph and equality on the right if and only if G is a matching of m edges. The lower bound in (6) follows in a straightforward way from (2) and (3):

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

The upper bound in (6) is proved as follows: The largest number of vertices of a graph with m edges (and no isolated vertices) is $2m$ and mK_2 uniquely attains this. So from (4) we obtain

$$E(G) \leq \sqrt{2mn} \leq \sqrt{2m \cdot 2m} = 2m.$$

Remark: This lower bound can be improved if G has a relatively large number of edges, specifically if $n^2/4 < m \leq n(n-1)/2$, by the inequality

$$E(G) \geq \frac{4m}{n}.$$

A lower bound for the energy of a graph solely in terms of its number of vertices is (see [4] for a proof):

$$E(G) \geq 2\sqrt{n-1},$$

with equality if and only G is the star $K_{1,n-1}$.

Thus *the star $K_{1,n-1}$ uniquely has the smallest energy among all graphs with n vertices (none of which are isolated).*

There are numerous other bounds on the energy of a graph usually under the assumption of some specific structure.

3 Hyperenergetic graphs

The complete graph K_n has eigenvalues $n-1$ and -1 ($n-1$ times). At one time it was thought that the complete graph K_n had the largest energy among all n vertex graphs G, that is,

$$E(G) \leq 2(n-1) \text{ with equality iff } G = K_n.$$

Godsil in the early 1980s constructed an example of a graph on n vertices whose energy exceeds $2(n-1)$. Now graphs G whose energy satisfies $E(G) > 2(n-1)$ are called *hyperenergetic*. The simplest construction of a family of hyperenergetic graphs is due to Walikar, Ramane, and Hampiholi:

The line graph $L(K_n)$ of K_n is hyperenergetic for $n \geq 5$.

It's worth seeing the outline of this simple proof: If G is a regular graph of degree r, then the characteristic polynomial of $L(G)$ can be given in terms of that of G:

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

Since $\phi_{K_n}(x) = (x-n+1)(x+1)^{n-1}$, we get that

$$E(L(K_n)) = 2n^2 - 6n > n^2 - n - 2 = E(K_{n(n-1)/2}) \quad (n \geq 5).$$

Since the line graph of K_n has $n(n-1)/2$ vertices, it does not furnish a hyperenergetic graph for all n. Gutman and Zhang constructed hyperenergetic graphs of all orders $n \geq 9$ by removing edges forming a star from K_n. An example of a hyperenergetic graph is also know for $n = 8$.

There are a number of other recent results on hyperenergetic graphs:

1. Balakrishnan [1] showed that if G is a regular graph of degree k, then

$$E(G) \leq k + \sqrt{k(n-1)(n-k)}$$

and this bound is sharp (e.g. it holds for K_n). He also showed that for each $r \geq 3$, there exists a pair of equienergetic (same energy) graphs of order $n = 4r$ that are not cospectral. There are several other constructions, of classes of equienergetic, non-cospectral graphs [2, 11, 12].

2. Answering a question in [1], Stevanović and I. Stanković showed that the graph $K_n - H$ obtained from K_n by deleting the edges of a Hamilton cycle H is hyperenergetic for n sufficiently large. They also showed that many circulant graphs (graphs with an adjacency matrix equal to a circulant) are hyperenergetic.

3. Yu and Lv [16] showed that among all trees with k pendent vertices, the tree with minimum energy is uniquely $P_{n,k}$ obtained from a path with $n - k + 1$ vertices by attaching $k - 1$ pendent vertices on one of its ends.

4. Using Gaussian sums, Shparlinski [13] gave constructions of circulant graphs with high energy.

5. Rada and Tineo [9] investigated polygonal chains with minimum energy.

6. Gutman and Zhou [5] defined the *Laplacian energy* of a graph using its Laplacian matrix $D - A$, where A is the adjacency matrix and D is the diagonal matrix of degrees:

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

where $\mu_1, \mu_2, \ldots, \mu_n$ are the (Laplacian) eigenvalues of $D - A$, m is the number of edges of G, and $2m/n$ is the average degree of a vertex of G. Regular graphs have the same energy as their line graphs. It is not yet clear whether Laplacian energy is a fruitful concept.

4 Maximal energy

Recall that we are assuming that G is a graph with n vertices and m edges and that G has no isolated vertices (thus $2m \geq n$).

The following upper bound on energy is from [7].

$$E(G) \leq \frac{2m}{n} + \sqrt{(n-1)\left(2m - \left(\frac{2m}{n}\right)^2\right)}. \tag{7}$$

Equality holds in (7) if and only if G is either $(n/2)K_2$, the complete graph K_n, or certain strongly regular graphs.

To prove (7), observe that the adjacency matrix of G has average row sum equal to $2m/n$ and hence $\lambda_1 \geq 2m/n$. By (3), it follows that

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

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

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

Hence

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

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 $2m \geq n$, $\sqrt{2m/n} \leq 2m/n \leq \lambda_1$. Hence $F(\lambda_1) \leq F(2m/n)$ from which (7) follows. For the case of equality in (7), see [7].

It can be shown that (7) is at least as good as (5).

An improvement of the bound (5) for energy in terms only of the number n of vertices is [7]:

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

with equality holding if and only if a strongly regular graph with parameters $(n, k = (n+\sqrt{n})/2, \lambda = (n+2\sqrt{n})/4, \mu = (n+2\sqrt{n})/4)$ exists. (So this shows that a graph can have energy of order $n^{3/2}$ while K_n has energy of order n. Note that the largest eigenvalue of K_n is $\lambda_1 = n-1$; the largest eigenvalue of these strongly regular graphs is $\lambda_1 = k = (n+\sqrt{n})/2$.) The inequality (8) follows from (7) by observing that the right hand side of (7), as a function of m, $m \geq n/2$, is maximized when

$$m = \frac{n^2 + n\sqrt{n}}{4} = \frac{n^2 + n^{3/2}}{4}$$

and then substituting this value into (7). Note that K_n has $n(n-1)/2$ edges and

$$\lim_{n\to\infty} \frac{n(n-1)/2}{(n^2+n^{3/2})/4} = 2.$$

This suggests to look for high energy graphs among graphs with about half as many edges as K_n. A family of strongly regular graphs with $n = 2^{2t+4}$ and degree of regularity $k = (2^{t+1}-1)(2^{t+2}-1)) \approx 2^{2t+3} = n/2$ attaining the bound (7) is shown to exist in [7].

In [8] and [10], high energy bipartite graphs are investigated with results similar to those for the non-bipartite case. The following bounds are derived:

(1) [8] If G is a bipartite graph with $n > 2$ vertices and $m \geq n/2$ edges, then

$$E(G) \leq 2\left(\frac{2m}{n}\right) + \sqrt{(n-2)\left(2m - 2\left(\frac{2m}{n}\right)^2\right)}. \quad (9)$$

Equality is characterized.

(2) [8] If G is a bipartite graph with $n > 2$ vertices, then

$$E(G) \leq \frac{n}{\sqrt{8}}(\sqrt{n}+\sqrt{2}) \quad (10)$$

with equality if and only if $n = 2v$ and G is the incidence graph of a 2-$(v, k = \frac{v+\sqrt{v}}{2}, \lambda = \frac{v+2\sqrt{v}}{4})$-design. Here by the *incidence graph* is meant the graph with adjacency matrix

$$A = \begin{bmatrix} O & B \\ B^T & O \end{bmatrix}$$

where B is the point-block incidence matrix of the design. A family of maximal energy bipartite graphs is obtained by taking B to be the adjacency matrix of a maximal energy graph.

(3) [10] If G is a bipartite graph with n vertices and m edges, then an upper bound for $E(G)$ is given in terms of n, m, and the 4th spectral moment $M_4 = \sum_{i=1}^{n} \lambda_i^4$. Note that $M_1 = 0, M_2 = 2m$ and $M_k = 0$ for k odd if G is bipartite. If G is regular, equality holds in this bound if and only if G is the incidence graph of a symmetric block design.

5 Basic problems

The following seem to be the unsolved basic problems:

1. What is the maximum energy of a graph on n vertices? (cf. (8))

2. What are the graphs with maximum energy? How can they be constructed?

3. Is there some graph structure that guarantees high energy?

4. How, if at all, is the degree sequence of a graph related to graph structure?

5. As pointed out in [4] (and it follows from the interlacing inequalities)

$$E(G') \leq E(G) \quad (G' \text{ an induced subgraph of } G).$$

   On the other hand, since K_n does not have maximum energ, it is **not** true in general that

$$E(G') \leq E(G) \quad (G' \text{ a spanning subgraph of } G).$$

   When does this inequality hold? In particular, when does it hold when G' is obtained from G by removing an edge? Do there exist graphs such that removing any edge increases the energy?

6. Hyperenergetic graphs of order n are graphs whose energy is greater than the energy of the complete K_n. Since K_n has largest eigenvalue (spectral radius) $n - 1$ and is the unique graph with this spectral radius), how large can the spectral radius of a hyperenergetic graph be? In fact, as discussed following (8) the maximal energy graphs have spectral radius equal to $(n + \sqrt{n})/2$.

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