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ENERGY OF A GRAPH *

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Abstract

The energy of a graph is the sum of the absolute values of its eigenvalues. It is used in chemistry to approximate the total π-electron energy of molecules. In this paper we present upper bounds for the energy of a graph in terms of its degree sequence, and characterize those maximal energy graphs and maximal energy bipartite graphs.

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Given a graph G with n vertices, define the *energy* of G, denoted $E(G)$, by

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

where $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$ are the eigenvalues of G. This concept was introduced in the subject of chemistry by I. Gutman and is intensively studied since it can be used to approximate the total π-electron of a molecule (see [1, 2], for example). Recently, Koolen and Moulton [6, 7] showed that for a graph G with n vertices and m edges

$$E(G) \leq \frac{2m}{n} + \sqrt{(n-1)\left(2m - \frac{4m^2}{n^2}\right)} \tag{1}$$

and for a bipartite graph with n vertices and m edges

$$E(G) \leq \frac{4m}{n} + \sqrt{(n-2)\left(2m - \frac{8m^2}{n^2}\right)}, \tag{2}$$

and characterized those graphs for which these bounds are best possible (see [5], where the above bounds were published for the first time). Then for a graph G with n vertices

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

and for a bipartite graph G with n vertices

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

and those graphs for which these bounds are best possible can be characterized [6, 7].

A graph G is *semiregular bipartite* (of degrees r_1 and r_2) if it is bipartite and each vertex in the same part of bipartition has the same degree (each vertex in one part of bipartition has degree r_1 and each vertex in the other part of bipartition has degree r_2). Clearly a regular bipartite graph is a semiregular bipartite graph ($r_1 = r_2$).

Among the known lower bounds for λ_1 is the following [8]:

$$\lambda_1 \geq \sqrt{\frac{\sum_{i=1}^{n} d_i^2}{n}},$$

and equality holds if and only if G is a regular graph or a semiregular bipartite graph, where $d_1, d_2, \ldots, d_n$ is the degree sequence of G.

A *strongly regular graph* G with parameters (n, k, ρ, σ) is a k-regular graph on n vertices, each pair of adjacent vertices has ρ common neighbours and each pair of non-adjacent vertices has σ common neighbours. If $\sigma \geq 1$ and G is non-complete, then the eigenvalues of G are k, s and t with multiplicities $1, m_s$ and m_t, where s, t are the roots of $x^2 + (\sigma - \rho)x + (\sigma - k) = 0$, and m_s and m_t can be determined by $m_s + m_t = n - 1$ and $k + m_s s + m_t t = 0$.

We first give an upper bound for the energy of a graph with n vertices, m edges and degree sequence $d_1, d_2, \ldots, d_n$, and characterize those graphs for which this bound is best possible.

Theorem 1 *If G is a graph with n vertices, m edges and degree sequence $d_1, d_2, \ldots, d_n$, then*

$$E(G) \leq \sqrt{\frac{\sum_{i=1}^n d_i^2}{n}} + \sqrt{(n-1)\left(2m - \frac{\sum_{i=1}^n d_i^2}{n}\right)}. \tag{3}$$

Moreover, equality in (3) holds if and only if G is either $\frac{n}{2}K_2$ $(n = 2m)$, K_n $(m = n(n-1)/2)$, a non-complete connected strongly regular graph with two non-trivial eigenvalues both with abosulate value $\sqrt{(2m - (\frac{2m}{n})^2)/(n-1)}$, or nK_1 $(m = 0)$.

Proof. Recall that [8]

$$\lambda_1 \geq \sqrt{\frac{\sum_{i=1}^n d_i^2}{n}}.$$

By the Cauchy-Schwartz inequality,

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

Hence

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

Note that the function $F(x) = x + \sqrt{(n-1)(2m-x^2)}$ decreases for $\sqrt{2m/n} \le x \le \sqrt{2m}$, and $\sqrt{2m/n} \le \sqrt{(\sum_{i=1}^{n} d_i^2)/n} \le \lambda_1$, we see that $F(\lambda_1) \le F\left(\sqrt{(\sum_{i=1}^{n} d_i^2)/n}\right)$. This proves (3).

It is easy to check that if G is one of the graphs given in the second part of the theorem, then equality in (3) holds.

Conversely, if equality in (3) holds, then by the above argument, we see that $\lambda_1 = \sqrt{(\sum_{i=1}^{n} d_i^2)/n}$. It follows that G is a regular graph or a semiregular bipartite graph. If G is regualr and $m > 0$, then $\lambda_1 = \sqrt{(\sum_{i=1}^{n} d_i^2)/n} = 2m/n$, and hence 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 abosulate value $\sqrt{(2m - (\frac{2m}{n})^2)/(n-1)}$ [6]; If $m = 0$, then G is nK_1. Now suppose G is a semiregular bipartite graph. Since equality holds in the Cauchy-Schwartz inequality given above, we have $\sqrt{(\sum_{i=1}^{n} d_i^2)/n} = \lambda_1 = -\lambda_n = \sqrt{(2m - \lambda_1^2)/(n-1)}$, from which we have $\sum_{i=1}^{n} d_i^2 = 2m$, and hence $d = 1$ or 0 for $1 \le i \le n$. Thus G is either $\frac{n}{2}K_2$ or nK_1. □

Remark 1 Note that $\sqrt{(\sum_{i=1}^{n} d_i^2)/n} \ge 2m/n$ (since $4m^2 = (\sum_{i=1}^{n} d_i)^2 \le n\sum_{i=1}^{n} d_i^2$) and $F(x) = x + \sqrt{(n-1)(2m-x^2)}$ decreases for $\sqrt{2m/n} \le x \le \sqrt{2m}$. We have

$$E(G) \le F\left(\sqrt{(\sum_{i=1}^{n} d_i^2)/n}\right) \le F(2m/n).$$

$E(G) \le F(2m/n)$ is (1).

To investigate the energy of a bipartite graph, we need the following lemma.

Lemma 1 *Let G be a connected bipartite graph with n vertices and m edges, and let $d_1, d_2, \ldots, d_n$ be the degree sequence of G. Then*

$$d_1^2 + d_2^2 + \cdots + d_n^2 \le mn,$$

equality holds if and only if G is a complete bipartite graph.

Proof. Let E be the edge set of G. For any edge uv of G, $d_u + d_v \leq n$. Then $\sum_{i=1}^{n} d_i^2 = \sum_{uv\in E}(d_u + d_v) \leq mn$. The equality holds if and only if $d_u + d_v = n$ for any edge uv of G, i.e., G is complete bipartite. □

Recall that a 2-(v, k, λ)-design is a collection of k-subsets or blocks of a set of v points, such that each 2-set of the points lies in exactly λ blocks. It is known that $bk(k-1) = \lambda v(v-1)$. If $b = v$, then the design is called *symmetric*. The *incidence matrix* of a 2-(v, k, λ)-design is a $v \times b$ matrix $B = [b_{ij}]$ where $b_{ij} = 1$ if the i-th point is contained in the j-th block, and $b_{ij} = 0$ otherwise. The *incidence graph* of a design is defined to be the graph with adjacency matrix

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

The incidence graph of a 2-(v, k, λ)-design with $v > k > \lambda > 0$ (and then by Fisher's inequality, $b \geq v$) has eigenvalues $\sqrt{rk}$, $\sqrt{r-\lambda}$, 0, $-\sqrt{r-\lambda}$, $-\sqrt{rk}$ with multiplicities $1, v-1, b-v, v-1$ and 1, where $r = bk/v$ is the number of blocks containing a given point (for more details, see [3]). The incidence graph of a 2-(v, k, λ)-design is a semiregular bipartite graph of degrees r and k with $v + b$ vertices and $vr(= bk)$ edges.

Next we give an upper bound for the energy of a bpartite graph with n vertices, m edges and degree sequence $d_1, d_2, \ldots, d_n$, and characterize those graphs for which this bound is best possible.

Theorem 2 *If G is a bipartite graph with $n > 2$ vertices, m edges and degree sequence $d_1, d_2, \ldots, d_n$, then*

$$E(G) \leq 2\sqrt{\frac{\sum_{i=1}^{n} d_i^2}{n}} + \sqrt{(n-2)\left(2m - \frac{2\sum_{i=1}^{n} d_i^2}{n}\right)}. \tag{4}$$

Moreover, equality in (4) holds if and only if G is either $\frac{n}{2}K_2$ $(n = 2m)$, $K_{r,n-r}$ with $1 \leq r \leq n/2$ $(m = r(n-r))$, the incidence graph of a symmetric 2-(v, k, λ)-design with $v > k$, $k = 2m/n$ and $\lambda = k(k-1)/(v-1)$ $(n = 2v)$, or nK_1 $(m = 0)$.

Proof. Recall that [8]

$$\lambda_1 \geq \sqrt{\frac{\sum_{i=1}^{n} d_i^2}{n}}.$$

By the Cauchy-Schwartz inequality,

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

Hence

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

Note that the function $H(x) = 2x + \sqrt{(n-2)(2m-2x^2)}$ decreases for $\sqrt{2m/n} \leq x \leq \sqrt{m}$, and $\sqrt{2m/n} \leq \sqrt{(\sum_{i=1}^{n} d_i^2)/n} \leq \lambda_1$, we see that $H(\lambda_1) \leq H\left(\sqrt{(\sum_{i=1}^{n} d_i^2)/n}\right)$. This proves (4).

It is easy to check that if G is one of the graphs given in the second part of the theorem, then equality in (4) holds.

Conversely, if equality in (4) holds, then by the above argument, we see that $\lambda_1 = \sqrt{(\sum_{i=1}^{n} d_i^2)/n}$. It follows that G is a semiregular bipartite graph. Since equality holds in the Cauchy-Schwartz inequality given above, we have $|\lambda_i| = \sqrt{(2m-2\lambda_1^2)/(n-2)}$ for $2 \leq i \leq n-1$. Hence we have the following possibilities: either G has two eigenvalues with equal absolute values and hence $G = mK_2$, G has three distinct eigenvalues, i.e., $\lambda_i = 0$ for $2 \leq i \leq n-1$, and hence $(\sum_{i=1}^{n} d_i^2)/n = \lambda_1^2 = m$ and by Lemma 1 $G = K_{r,n-r}$ with $1 \leq r \leq n/2$, G has four distinct eigenvalues in which case G is regular (since 0 is not an eigenvalue and G is a semiregular bipartite graph) and connected, $\lambda_1 = 2m/n > \sqrt{(2m-2\lambda_1^2)/(n-2)}$ and hence G is the incidence graph of a symmetric 2-$(v, 2m/n, \lambda)$-design [4], or $G = nK_1$ $(m = 0)$. □

Remark 2 As in Remark 1, note that $\sqrt{(\sum_{i=1}^{n} d_i^2)/n} \geq 2m/n$ and $H(x) = 2x + \sqrt{(n-2)(2m-2x^2)}$ decreases for $\sqrt{2m/n} \leq x \leq \sqrt{m}$. For a bipartite graph G, we have

$$E(G) \leq H\left(\sqrt{(\sum_{i=1}^{n} d_i^2)/n}\right) \leq H(2m/n).$$

$E(G) \leq H(2m/n)$ is (2).

Remark 3 Let G is a bipartite graph with $n > 2$ vertices, m edges and degree sequence $d_1, d_2, \ldots, d_n$, where n is odd. By the Cauchy-Schwartz inequality ($t = (n-1)/2$, $\lambda_{t+1} = 0$),

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

Hence

$$E(G) \leq 2\lambda_1 + \sqrt{(n-3)(2m-2\lambda_1^2)}.$$

There are two cases:

Case 1: $(\sum_{i=1}^{n} d_i^2)/n \geq 2m/(n-1)$. Since the function $I(x) = 2x + \sqrt{(n-3)(2m-2x^2)}$ decreases for $\sqrt{2m/(n-1)} \leq x \leq \sqrt{m}$ and $\sqrt{2m/(n-1)} \leq \sqrt{(\sum_{i=1}^{n} d_i^2)/n} \leq \lambda_1$, we see that $I(\lambda_1) \leq I\left(\sqrt{(\sum_{i=1}^{n} d_i^2)/n}\right)$. This proves

$$E(G) \leq 2\sqrt{\frac{\sum_{i=1}^{n} d_i^2}{n}} + \sqrt{(n-3)\left(2m - \frac{2\sum_{i=1}^{n} d_i^2}{n}\right)}. \tag{5}$$

It is not difficult to see that equality in (5) holds if $G = K_{r,n-r}$ with $1 \leq r < n/2$, or G is the incidence graph of a 2-(v, k, λ)-design [3] with

$$k > \lambda, \lambda = \frac{k(k-1)}{v(v-1)}(v+1) \text{ and } n = 2v+1,$$

or $G = nK_1$.

Case 2: $(\sum_{i=1}^{n} d_i^2)/n < 2m/(n-1)$. Then $4m^2/n^2 \leq (\sum_{i=1}^{n} d_i)^2/n^2 < 2m/(n-1)$ and hence $2m \leq n+1$. We claim that $2m \neq n+1$. Otherwise, suppose $2m = n+1$. Then $\sum_{i=1}^{n} d_i^2 < 2mn/(n-1) = n+2+2/(n-1)$, from which we have $\sum_{i=1}^{n} d_i^2 \leq n+2$. It follows that either $\sum_{i=1}^{n} d_i^2 = n+1 = 2m$ and hence $d_i \leq 1$ for all i, which is impossible, or $\sum_{i=1}^{n} d_i^2 = n+2$ and hence $\sum_{i=1}^{n} d_i(d_i-1) = 1$, which is also impossible since $\sum_{i=1}^{n} d_i(d_i-1)$ is even. Hence $2m \neq n+1$. Then $2m \leq n-1$, $E(G) \leq H(1) = 2m$ (which also follows from [6, Theorem 2], and equality holds if G is the disjoint union of mK_2 and $(n-2m)K_1$ with $1 \leq m < n/2$.

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