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Relation Between Energy and Extended Energy of a Graph

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Abstract

Let d_i denote the degree of the vertex v_i of the graph G. The extended adjacency matrix of G is constructed by assigning the weight $\frac{1}{2}\left(\frac{d_i}{d_j}+\frac{d_j}{d_i}\right)$ to the edge connecting the vertices v_i and v_j. The extended energy of G is the sum of absolute values of the eigenvalues of the extended adjacency matrix. We prove that the extended graph energy of a bipartite graph is not smaller than its ordinary energy, and conjecture that the results holds also for non-bipartite graphs.

Key Words: energy (of graph), extended energy, degree (of vertex), spectrum (of graph), eigenvalue (of graph).

AMS Classification: 05C50, 05C07

1 Introduction

Within spectral graph theory [1, 2] it is customary to consider the eigenvalues of the adjacency matrix. For a graph G with vertices $v_1, v_2, \ldots, v_n$, the adjacency matrix $\mathbf{A}(G)$ is a square matrix of order n, whose (i,j)-entry is equal to

$$a_{ij} = \begin{cases} 0 & \text{if } i = j \\ 1 & \text{if the vertices } v_i \text{ and } v_j \text{ are adjacent} \\ 0 & \text{if the vertices } v_i \text{ and } v_j \text{ are not adjacent.} \end{cases}$$

The characteristic polynomial of $\mathbf{A}(G)$ is referred to as the characteristic polynomial of the graph G. The eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ of $\mathbf{A}(G)$ form the spectrum of the graph G. An important, and much studied spectrum–based invariant is the *graph energy*, defined as

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

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Details of the theory of graph energy are found in the monograph [4] and the references cited therein.

In what follows, d_i will denote the degree (= number of first neighbors) of the vertex v_i of the graph G.

In 1994, Yang et al. [8] considered an extended version $\mathbf{A}_{ext}(G)$ of the adjacency matrix, defining its (i, j)-entry as

$$a_{ij}^{ext} = \begin{cases} 0 & \text{if } i = j \\ \frac{1}{2}\left(\frac{d_i}{d_j} + \frac{d_j}{d_i}\right) & \text{if the vertices } v_i \text{ and } v_j \text{ are adjacent} \\ 0 & \text{if the vertices } v_i \text{ and } v_j \text{ are not adjacent.} \end{cases}$$

If $\eta_1, \eta_2, \ldots, \eta_n$ are the eigenvalues of $\mathbf{A}_{ext}(G)$, then the respective *extended graph energy* is defined as [8]

$$\mathcal{E}_{ext} = \mathcal{E}_{ext}(G) = \sum_{i=1}^{n} |\eta_i| \,.$$

If the adjacent vertices v_i and v_j have equal degrees, then $a_{ij}^{ext} = 1$. If $d_i \neq d_j$, then $a_{ij}^{ext} > 1$. Therefore, if all edges of the graph G connect vertices of equal degrees, then $\mathbf{A}_{ext}(G) = \mathbf{A}(G)$, and, consequently, $\mathcal{E}_{ext}(G) = \mathcal{E}(G)$. Note that this happens if each component of G is a regular graph.

Yang et al. [8] demonstrated that the extended energy is well correlated with several physicochemical properties of a variety of organic compounds, including those of pharmacologic importance. On the other hand, not much is known on the mathematical properties of $\mathcal{E}_{ext}$. In a recent paper [3], lower and upper bounds for $\mathcal{E}_{ext}$ are established. However, the most obvious problem with regard to $\mathcal{E}_{ext}$, namely its relation to the ordinary graph energy $\mathcal{E}$, remained unanswered. It this paper we offer a partial answer to this question, by proving:

Theorem 1.1. If G is a bipartite graph, then $\mathcal{E}_{ext}(G) \geq \mathcal{E}(G)$. Equality holds if and only if all edges of G connect vertices of equal degrees. In particular, if G is connected, then equality holds if and only if G is a regular graph.

In order to prove Theorem 1.1, we need some preparations.

2 Preliminary considerations

Let

$$P(x) = \sum_{k \geq 0} c_k \, n^{n-k}$$

be a polynomial with all zeros real. Then its energy satisfies [5, 7]

$$\mathcal{E}(P) = \frac{1}{\pi} \int_0^\infty \frac{dx}{x^2} \ln \left[\left(\sum_{k \geq 0} (-1)^k \, c_{2k} \, x^{2k} \right)^2 + \left(\sum_{k \geq 0} (-1)^k \, c_{2k+1} \, x^{2k+1} \right)^2 \right] .$$

If the zeros of $P(x)$ are symmetric w.r.t. $x = 0$, i.e., if $c_{2k+1} = 0$ for all $k \geq 0$, then

$$\mathcal{E}(P) = \frac{2}{\pi} \int_0^\infty \frac{dx}{x^2} \ln \sum_{k \geq 0} (-1)^k \, c_{2k} \, x^{2k} \, .$$

As well known, a graph is bipartite if and only if it does not contain cycles of odd size. The characteristic polynomial of a bipartite graph is of the form [1, 2]

$$\phi(G, x) = \sum_{k \geq 0} c_{2k} \, x^{n-2k}$$

and, analogously, the characteristic polynomial of its extended adjacency matrix conforms to the relation

$$\phi_{ext}(G, x) = \sum_{k \geq 0} c_{2k}^{ext} \, x^{n-2k} \, .$$

Then

$$\mathcal{E}_{ext}(G) = \frac{2}{\pi} \int_0^\infty \frac{dx}{x^2} \ln \sum_{k \geq 0} (-1)^k \, c_{2k}^{ext} \, x^{2k} \, .$$

3 Proof of Theorem 1.1

Recall that a Sachs graph is a graph consisting of vertices of degree one and/or two, i.e., all its components are isolated edges and/or cycles [2, 6]. Apply the Sachs theorem to $\phi_{ext}(G, x)$ [2, 6]:

$$c_{2k}^{ext} = \sum_{s \in \mathcal{S}_{2k}(G)} (-1)^{p(s)} \, 2^{q(s)} w(s)$$

where s is a Sachs graph and $\mathcal{S}_{2k}(G)$ is the set of all $(2k)$-vertex Sachs graphs that are as subgraphs contained in the graph G. Further,

$$\begin{aligned} p(s) &= \text{number of components of } s \\ q(s) &= \text{number of cyclic components of } s \\ w(s) &= \text{weight of } s. \end{aligned}$$

Recall that $w(s)$ is equal to the product of the weights of all edges contained in s, where the weight of a particular edge is $\frac{1}{2}\left(\frac{d_i}{d_j} + \frac{d_j}{d_i}\right)$. For the considerations that follow, it is only important that $w(s) \geq 1$.

Let G be a bipartite graph, and let the Sachs graph $s \in \mathcal{S}_{2k}(G)$ contain α isolated edges, β_i cycles of size $4i+2$, and γ_i cycles of size $4i$. Then,

$$p(s) = \alpha + \sum_i \beta_i + \sum_i \gamma_i$$

and

$$2k = 2\alpha + \sum_i (4i+2)\beta_i + \sum_i (4i)\gamma_i \,.$$

Therefore,

$$k + p = 2\alpha + 2\sum_i i\beta_i + 2\sum_i i\gamma_i + 2\sum_i \beta_i + \sum_i \gamma_i$$

implying

$$k + p \equiv \sum_i \gamma_i \ (mod\ 2)\,.$$

In view of the above, the contribution of the sachs graph s to $(-1)^k\, c_{2k}^{ext}$ is:

positive	if s contains no cycles of size divisible by 4
negative	if s contains one cycle of size divisible by 4
positive	if s contains two cycles of size divisible by 4
$\cdots$	$\cdots$
positive	if s contains an even number of cycles of size divisible by 4
negative	if s contains an odd number of cycles of size divisible by 4.

Suppose first that $\sum_i \gamma_i$ is zero or even. Then the contribution of the Sachs graph $s \in \mathcal{S}_{2k}(G)$ to $\mathcal{E}_{ext}(G)$ is positive, and because of $w(s) \geq 1$, it is not smaller than the respective contribution of s to $\mathcal{E}(G)$.

In this case, $\mathcal{E}_{ext}(G) \geq \mathcal{E}(G)$, with equality if all edges of G connect vertices of equal degree. Thus, if G is connected, equality holds if and only if G is a regular graph.

Remains the case when $\sum_i \gamma_i$ is an odd integer.

Then s has at least one cycle whose size is divisible by 4. Let, for the sake of simplicity, this be an 8-membered cycle, see Fig. 1.

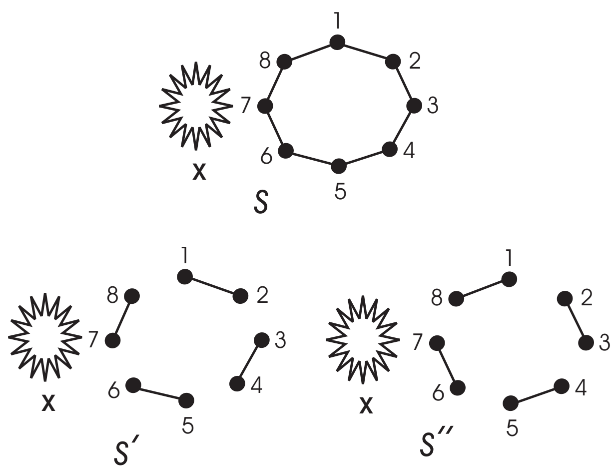

Fig. 1. A Sachs graph s containing an 8-membered cycle, and two Sachs graphs s' and s'' in which the 8-membered cycle is replaced by isolated edges. By X is indicated the other components of s, s', and s''.

Then, in addition to s, there exist two more Sachs graphs $s', s'' \in \mathcal{S}_{2k}(G)$, depicted in Fig. 1. Using the abbreviation

$$d_{ij} = \frac{1}{2}\left(\frac{d_i}{d_j} + \frac{d_j}{d_i}\right)$$

the total contribution of s, s', and s'' to $(-1)^k\, c_{2k}^{ext}$ is equal to:

$$\Big\{ -2d_{12}\, d_{23}\, d_{34}\, d_{45}\, d_{56}\, d_{67}\, d_{78}\, d_{81} \Big\} + \Big\{ d_{12}^2\, d_{34}^2\, d_{56}^2\, d_{78}^2 \Big\} + \Big\{ d_{23}^2\, d_{45}^2\, d_{67}^2\, d_{81}^2 \Big\}$$

plus the (necessarily positive) contribution coming from the fragments X. Evidently, the above expressions is equal to

$$\Big(d_{12}\, d_{34}\, d_{56}\, d_{78} - d_{23}\, d_{45}\, d_{67}\, d_{81} \Big)^2$$

which is positive or zero.

Thus, the joint contribution of the Sachs graphs s, s', and s'' to $\mathcal{E}_{ext}(G)$ is positive and not smaller that their contributions to $\mathcal{E}(G)$.

This completes the proof of Theorem 1.1.

4 Concluding Remarks

If the graph G is not bipartite, then it contains odd cycles. If a Sachs graph $s \in \mathcal{S}_{2k}(G)$ contains odd cycles, then their number must be even.

Consider the case when s contains two cycles of size $4\ell+1$ and no cycle of size divisible by 4. Then

$$p(s) = \alpha + \sum_i \beta_i + 2$$

and

$$2k = 2\alpha + \sum_i (4i+2)\beta_i + 2(4\ell+1)\,.$$

Therefore,

$$k + p = 2\alpha + 2\sum_i i\beta_i + 2\sum_i \beta_i + 4\ell + 3$$

implying

$$k + p \equiv 1 \ (mod\ 2)\,.$$

Therefore, the contribution of the Sachs graph s to $(-1)^k\, c_{2k}^{ext}$ is negative. In the general case, this (negative) contribution cannot be compensated by positive contributions of other Sachs graphs (as in the earlier considered case $\sum_i \gamma_i = \text{odd}$).

Analogous difficulties would be encountered in the study of the term $\sum_{k\geq 0} c_{2k+1}^{ext}\, x^{2k+1}$ which is present in the expression for $\mathcal{E}_{ext}(G)$ if G is non-bipartite.

For the above specified reasons, the present proof of Theorem 1.1 cannot be extended to non-bipartite graphs. We, nevertheless state the following:

If G is any graph, then $\mathcal{E}_{ext}(G) \geq \mathcal{E}(G)$. Equality holds if and only if all edges of G connect vertices of equal degrees. In particular, if G is connected, then equality holds if and only if G is a regular graph.

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