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Energy of Graphs with Self-Loops

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Abstract

The energy of graphs containing self-loops is considered. If the graph G of order n contains σ self-loops, then its energy is defined as $E(G) = \sum |\lambda_i - \sigma/n|$ where $\lambda_1, \lambda_2, \dots, \lambda_n$ are the eigenvalues of the adjacency matrix of G. Some basic properties of $E(G)$ are established, and several open problems pointed out or conjectured.

1 Introduction

A graph is said to be simple (or schlicht) if it does not possess directed, weighted or multiple edges, and self-loops [12,13,21]. Let G be a simple graph of order n, with vertex set $\mathbf{V} = \{v_1, v_2, \dots, v_n\}$. Its adjacency matrix $\mathbf{A}(G)$ is a square symmetric matrix of order n whose (i, j)-element is defined as

$$\mathbf{A}(G)_{ij} = \begin{cases} 1 & \text{if the vertices } v_i \text{ and } v_j \text{ are adjacent,} \\ 0 & \text{if the vertices } v_i \text{ and } v_j \text{ are not adjacent,} \\ 0 & \text{if } i = j. \end{cases}$$

Let $\lambda_1(G), \lambda_2(G), \dots, \lambda_n(G)$ be the eigenvalues of $\mathbf{A}(G)$. Then the energy of G is

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

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The theory of graph energy is nowadays a well elaborated field of applied mathematics and mathematical chemistry [14, 18]. One should recall that the concept of graph energy has a chemical origin and a chemical interpretation [8].

There are more than a thousand papers on graph energy and its variants [9, 10]. Practically all these papers are concerned with simple graphs. It is remarkable that the energy of graph with self-loops has not been considered so far. This is additionally surprising because graphs with self-loops (representing heteroatoms) are of evident chemical significance, and were much studied in the past, including their spectral properties [1, 5, 6, 15, 16, 19].

Let $\mathbf{S}$ be a subset of $\mathbf{V}(G)$. The number of elements of $\mathbf{S}$ will be denoted by σ.

Let G_S be the graph obtained from the simple graph G, by attaching a self-loop to each of its vertices belonging to $\mathbf{S}$. Then the adjacency matrix of G_S is a symmetric square matrix $\mathbf{A}(G_S)$ of order n, whose (i,j)-element is defined as

$$\mathbf{A}(G_S)_{ij} = \begin{cases} 1 & \text{if the vertices } v_i \text{ and } v_j \text{ are adjacent,} \\ 0 & \text{if the vertices } v_i \text{ and } v_j \text{ are not adjacent,} \\ 1 & \text{if } i = j \text{ and } v_i \in \mathbf{S}, \\ 0 & \text{if } i = j \text{ and } v_i \notin \mathbf{S}. \end{cases}$$

Let $\lambda_1(G_S), \lambda_2(G_S), \ldots, \lambda_n(G_S)$ be the eigenvalues of $\mathbf{A}(G_S)$. These all are real-valued, and

$$\sum_{i=1}^{n} \lambda_i(G_S) = \sigma \,. \tag{2}$$

Therefore, the energy of G_S (in full analogy to the energy of any matrix with non-zero diagonal [2, 3, 11]) has to be defined as

$$E(G_S) = \sum_{i=1}^{n} \left| \lambda_i(G_S) - \frac{\sigma}{n} \right| \tag{3}$$

In this paper, we begin to examine the properties of $E(G_S)$.

2 Basic properties of energy of graphs with self-loops

First we state an elementary result:

Lemma 1. *(a) If $\sigma = 0$, then $E(G_S) = E(G)$.*

(b) If $\sigma = n$, then $E(G_S) = E(G)$.

Proof. Lemma 1(a) is trivially obvious, since for $\sigma = 0$, the graphs G_S and G coincide.

Let $\mathbf{I}_n$ denote the unit matrix of order n. If $\sigma = n$, then $\mathbf{A}(G_S) = \mathbf{A}(G) + \mathbf{I}_n$. Therefore, $\lambda_i(G_S) = \lambda_i(G) + 1$, $i = 1, 2, \ldots, n$. Lemma 1(b) follows then from Eqs. (1) and (3). ■

Lemma 1 immediately leads to the question: What is the relation between $E(G_S)$ and $E(G)$ in the case of $1 \leq \sigma \leq n-1$? Based on our numerical studies, we state the following claim:

Conjecture 2. *Let G be any simple graph of order n, and $\mathbf{S}$ any subset of its vertices, $1 \leq \sigma \leq n-1$. Then $E(G_S) > E(G)$.*

If this conjecture is true, then we are faced with many further questions. For instance, for a given graph (or class of graphs), for which $\mathbf{S}$ is the difference $E(G_S) - E(G)$ maximal? Etc. etc.

Some simple examples, illustrating Conjecture 2 are collected in Table 1.

$\mathbf{S}$	$E(G_S)$
$\emptyset$	4.4721
$\{v_1\}$	4.7588
$\{v_2\}$	4.6659
$\{v_1, v_2\}$	4.6056
$\{v_1, v_3\}$	4.9770
$\{v_1, v_4\}$	4.8284
$\{v_2, v_3\}$	4.8284
$\{v_1, v_2, v_3\}$	4.7588
$\{v_1, v_2, v_4\}$	4.6659
$\{v_1, v_2, v_3, v_4\}$	4.4721

Table 1. Energies of the path P_4 with self-loops.

From Table 1 we see that the energy depends not only on the number of self-loops, but also on their position. We, however, observe that the energies of some different graphs coincide. This is the consequence of the following general result.

Theorem 3. *Let G be a bipartite graph of order n, with vertex set $\mathbf{V}$. Let $\mathbf{S}$ be a subset of $\mathbf{V}$. Then $E(G_S) = E(G_{V \setminus S})$.*

Proof. We prove Theorem 3 assuming that n is even. If n is odd, the proof would proceed in a fully analogous manner.

For the proof of Theorem 3, we need to recall details of the Sachs coefficient theorem [1,4,7,20].

Let $\phi(G_S,\lambda) = \det\left[\lambda\,\mathbf{I}_n - \mathbf{A}(G_S)\right]$ be the characteristic polynomial of G_S. We write it in the form

$$\phi(G_S,\lambda) = \phi_e(G_S,\lambda) + \phi_o(G_S,\lambda) \tag{4}$$

where

$$\phi_e(G_S,\lambda) = \sum_{k\geq 0} c_{2k}\,\lambda^{n-2k} \qquad \text{and} \qquad \phi_o(G_S,\lambda) = \sum_{k\geq 0} c_{2k+1}\,\lambda^{n-2k-1}\,.$$

Let $\mathbf{H}_k$ be the set of k-vertex subgraphs of G_S whose components are cycles and/or copies of P_2 and/or isolated vertices with self-loops. According to the Sachs theorem,

$$c_k = \sum_{H\in\mathbf{H}_k} (-1)^{p(H)}\,2^{c(H)} \tag{5}$$

where $p(H)$ is the number of components of H and $c(H)$ the number of cycles of H.

Since G_S is bipartite, all its cycles (if any) are of even size. Therefore, all subgraphs contained in H_{2k} must possess and even number (or zero) of vertices with self-loops. All components of H_{2k+1} must possess an odd number of vertices with self-loops.

Let G_S^- be the graph obtained from G_S by changing the signs of all its self-loops from +1 to -1. Then by the Sachs formula (5),

$$\phi(G_S^-,\lambda) = \phi_e(G_S,\lambda) - \phi_o(G_S,\lambda)\,.$$

Let ξ be a zero of the polynomial $\phi(G_S,\lambda)$. Then in view of Eq. (4),

$$\phi_e(G_S,\xi) = -\phi_o(G_S,\xi)\,.$$

In addition,

$$\phi_e(G_S,\xi) = \phi_e(G_S,-\xi) \qquad \text{and} \qquad -\phi_o(G_S,\xi) = \phi_o(G_S,-\xi)$$

implying

$$\phi_e(G_S,-\xi) - \phi_o(G_S,-\xi) = 0 \qquad \text{i.e.,} \qquad \phi(G_S^-,-\xi) = 0\,.$$

We thus conclude that if $\lambda_1(G_S),\lambda_2(G_S),\ldots,\lambda_n(G_S)$ are the eigenvalues of G_S, then $-\lambda_1(G_S),-\lambda_2(G_S),\ldots,-\lambda_n(G_S)$ are the eigenvalues of G_S^-.

Consider now the characteristic polynomial of $G_{V\setminus S}$.

Let $\mathbf{A}(G_S) = \mathbf{A}(G) + \mathbf{J}_S$ and $\mathbf{A}(G_{V\backslash S}) = \mathbf{A}(G) + \mathbf{J}_{V\backslash S}$, with $\mathbf{J}_S + \mathbf{J}_{V\backslash S} = \mathbf{I}_n$. Then

$$\begin{aligned}\phi(G_{V\backslash S},\lambda) &= \det\left[\lambda\,\mathbf{I}_n - \mathbf{A}(G) - \mathbf{J}_{V\backslash S}\right] = \det\left[\lambda\,\mathbf{I}_n - \mathbf{A}(G) - \mathbf{I}_n + \mathbf{J}_S\right] \\ &= \det\left[(\lambda-1)\,\mathbf{I}_n - (\mathbf{A}(G) - \mathbf{J}_S)\right] = \det\left[(\lambda-1)\,\mathbf{I}_n - \mathbf{A}(G_S^-\right]\end{aligned}$$

from which it follows

$$\phi(G_{V\backslash S},\lambda) = \phi(G_S^-,\lambda-1)\,.$$

This means that the eigenvalues $\lambda_i(G_{V\backslash S})\,,\ i=1,2,\ldots,n$, coincide with $\lambda_i(G_S^-)+1\,,\ i=1,2,\ldots,n$. Bearing this in mind, we have

$$\begin{aligned}E(G_{V\backslash S}) &= \sum_{i=1}^{n}\left|\lambda_i(G_{V\backslash S}) - \frac{n-\sigma}{n}\right| = \sum_{i=1}^{n}\left|\lambda_i(G_{V\backslash S}) - 1 + \frac{\sigma}{n}\right| \\ &= \sum_{i=1}^{n}\left|\lambda_i(G_S^-) + 1 - 1 + \frac{\sigma}{n}\right| = \sum_{i=1}^{n}\left|-\lambda_i(G_S) + \frac{\sigma}{n}\right| = \sum_{i=1}^{n}\left|\lambda_i(G_S) - \frac{\sigma}{n}\right|\,.\end{aligned}$$

Theorem 3 follows now by Eq. (3). ■

The equality $E(G_S) = E(G_{V\backslash S})$ does not hold if the graph G is not bipartite. The simplest example showing this is the triangle with one self-loop (whose energy is 4.1618) and with two self-loops (whose energy is 4.1308).

3 McClelland–type bound for the energy of graphs with self-loops

In this section we obtain a McClelland–type upper bound [17] for the energy of graphs with self-loops. In order to achieve this goal, we first establish a few auxiliary results.

Lemma 4. *Let G_S be a graph of order n, with m edges, and σ self-loops. Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be its eigenvalues. Then*

$$\sum_{i=1}^{n}\lambda_i^2 = 2m + \sigma\,.$$

Proof.

$$\begin{aligned}\sum_{i=1}^{n}\lambda_i^2 &= \sum_{i=1}^{n}\left[\mathbf{A}(G_S)^2\right]_{ii} = \sum_{i=1}^{n}\left[\left(\mathbf{A}(G) + \mathbf{J}_S\right)^2\right]_{ii} \\ &= \sum_{i=1}^{n}\left[\mathbf{A}(G)^2 + \mathbf{A}(G)\,\mathbf{J}_S + \mathbf{J}_S\,\mathbf{A}(G) + \mathbf{J}_S^2\right]_{ii}\,.\end{aligned}$$

By direct calculation it is easy to shown that

$$\sum_{i=1}^{n}\left[\mathbf{A}(G)^2\right]_{ii}=2m\quad,\quad\sum_{i=1}^{n}\left[\mathbf{A}(G)\,\mathbf{J}_S\right]_{ii}=\sum_{i=1}^{n}\left[\mathbf{J}_S\,\mathbf{A}(G)\right]_{ii}=0\quad,\quad\sum_{i=1}^{n}\left[\mathbf{J}_S^2\right]_{ii}=\sigma$$

from which Lemma 4 follows. ■

Lemma 5. *With the same notation as in Lemma 4,*

$$\sum_{i=1}^{n}\left|\lambda_i-\frac{\sigma}{n}\right|^2=2m+\sigma-\frac{\sigma^2}{n}$$

Proof.

$$\sum_{i=1}^{n}\left|\lambda_i-\frac{\sigma}{n}\right|^2=\sum_{i=1}^{n}\left(\lambda_i^2-2\lambda_i\frac{\sigma}{n}+\frac{\sigma^2}{n^2}\right)=\sum_{i=1}^{n}\lambda_i^2-2\,\frac{\sigma}{n}\sum_{i=1}^{n}\lambda_i+\frac{\sigma^2}{n}$$

and Lemma 5 follows by using Lemma 4 and formula (2). ■

Theorem 6. *Let G_S be a graph of order n, with m edges, and σ self-loops. Then*

$$E(G_S)\leq\sqrt{n\left(2m+\sigma-\frac{\sigma^2}{n}\right)}\,. \tag{6}$$

Proof. The expression

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\left(\left|\lambda_i-\frac{\sigma}{n}\right|-\left|\lambda_j-\frac{\sigma}{n}\right|\right)^2$$

is evidently non-negative. Expanding it we get

$$n\sum_{i=1}^{n}\left|\lambda_i-\frac{\sigma}{n}\right|^2+n\sum_{j=1}^{n}\left|\lambda_j-\frac{\sigma}{n}\right|^2-2\sum_{i=1}^{n}\left|\lambda_i-\frac{\sigma}{n}\right|\sum_{j=1}^{n}\left|\lambda_j-\frac{\sigma}{n}\right|$$

which by Lemma 5 and Eq. (3) yields

$$2n\left(2m+\sigma-\frac{\sigma^2}{n}\right)-2\,E(G_S)^2\geq 0$$

from which Theorem 6 directly follows. ■

As expected, formula (6) reduces to the original McClelland bound [17] for $\sigma=0$, but also for $\sigma=n$, in harmony with Lemma 1(b).

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