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Graph energy and nullity

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Abstract: The energy of a graph is the sum of absolute values of its eigenvalues. The nullity of a graph is the algebraic multiplicity of number zero in its spectrum. Empirical facts indicate that graph energy decreases with increasing nullity, but proving this property is difficult. In this paper, a method is elaborated by means of which the effect of nullity on graph energy can be quantitatively estimated.

Keywords: Energy of graph; Nullity of graph; Graph spectrum.

MSC: 05C50; 55C92.

1. Introduction

The concept of graph energy was introduced in 1978 [1], as a kind of generalization of the HMO total π-electron energy [2]. After a twenty-years period of silence, graph energy became a popular topic of research in chemical graph theory [3], with over than hundred papers published each year [4,5]. Of the numerous properties established for graph energy, one remains a long-time open problem. Namely, already in the early days of the study of graph energy and its predecessor total π-electron energy, it was observed that it somehow decreases with the increasing number of zero eigenvalues in the graph spectrum [2,6].

Let G be a (molecular) graph, possessing n vertices. Let $\lambda_1, \lambda_2 \ldots, \lambda_n$ be the eigenvalues of the $(0,1)$-adjacency matrix of G, forming the spectrum of G. Then the *energy* of G is defined as [1,3]:

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

whereas its *nullity*, denoted by $\eta = \eta(G)$, is equal to the number of zero eigenvalues (= the algebraic multiplicity of the number zero in the graph spectrum). Then the above mentioned regularity can be formally stated as follows.

Conjecture 1. *Let G and G' be two structurally similar graphs. Let $\eta(G) < \eta(G')$. Then $E(G) > E(G')$.*

The problem with this conjecture is that the meaning of "structurally similar graphs" is not clear and cannot be rigorously defined. Earlier attempts to justify its validity were based on designing approximate expression for $E(G)$, containing the term $\eta(G)$ [6–9], or by constructing a suitably chosen example for the graphs G, G' [10].

It this paper we elaborate a general method for quantifying the dependence of graph energy on nullity, in which the usage of the "structurally similar graph" G' is avoided.

2. Effect of nullity on the energy of a non-singular graph

Let G be a (molecular) graph as defined above, and assume that it is non-singular, i.e., that it has no zero eigenvalues, $\eta(G) = 0$. Let its characteristic polynomial be

$$\phi(G, \lambda) = \sum_{k=0}^{n} c_k \lambda^{n-k} = \prod_{i=1}^{n} (\lambda - \lambda_i),$$

and recall that

$$c_0 = 1 \ , \ c_1 = \sum_{i=1}^{n} \lambda_i = 0, \tag{1}$$

and

$$c_k = \sum_{1 \le i_1 < i_2 < \cdots < i_k \le n} \lambda_{i_1} \lambda_{i_2} \cdots \lambda_{i_k}, \tag{2}$$

for $k = 2, ..., n$. In particular,

$$c_n = \prod_{i=1}^{n} \lambda_i \neq 0.$$

Throughout this paper, since we are mainly interested in molecular graphs, it will be assumed that n is even, and that

$$\lambda_1 \ge \lambda_2 \ge \cdots \lambda_{n/2} > 0 > \lambda_{n/2+1} \ge \lambda_{n/2+2} \ge \cdots \ge \lambda_n \, .$$

If so, then $c_2 < 0$, $c_4 > 0$, $c_6 < 0$, $c_8 > 0$, ..., i.e.,

$$(-1)^k \, c_{2k} > 0 \ \text{ for all } k = 0, 1, 2, \ldots, n/2, \tag{3}$$

and

$$\sum_{k=0}^{n/2-1} (-1)^k \, c_{2k} \, x^{n-2k} > 0 \ \text{ for all } x \ge 0 \, . \tag{4}$$

The coefficients c_k are the structural parameters of the graph G on which its energy depends. It is known that [11–14]:

$$E(G) = Re \left[\frac{2}{\pi} \int_0^{\infty} \ln \sum_{k=0}^{n} c_k \, (ix)^{-k} \, dx \right] = \frac{2}{\pi} \int_0^{\infty} \ln \left| \sum_{k=0}^{n} c_k \, (ix)^{-k} \right| dx, \tag{5}$$

where $i = \sqrt{-1}$ and Re indicates the real part of a complex number. Recall that for any complex number z, $|z| \ge Re(z)$.

Our approach is based on the following. Instead of looking for a graph G' that would be "structurally similar" to G, we construct a quasi-spectrum, consisting of the numbers $\lambda'_1, \lambda'_2, \ldots, \lambda'_n$, that would be as similar as possible to the true spectrum of G, but that would contain a single zero element. Let $\lambda'_k \neq 0$ for $k = 1, 2, \ldots, n-1$ and $\lambda'_n = 0$, which is equivalent to the condition $\eta(G') = 1$. Then, in analogy to Equations (1) and (2), we define

$$c'_0 = 1 \ , \ c'_1 = \sum_{i=1}^{n} \lambda'_i = 0,$$

and

$$c'_k = \sum_{1 \le i_1 < i_2 < \cdots < i_k \le n} \lambda'_{i_1} \lambda'_{i_2} \cdots \lambda'_{i_k},$$

for $k = 2, ..., n$, implying that

$$c'_n = \prod_{i=1}^{n} \lambda'_i = 0 \, .$$

Bearing in mind Equation (5), we now construct an auxiliary quantity [15,16]:

$$E'(G) = \frac{2}{\pi} \int_0^{\infty} \ln \left| \sum_{k=0}^{n} c'_k \, (ix)^{-k} \right| dx \, .$$

By requiring that $c'_k = c_k$ for $k = 1, 2, \ldots, n-1$, it immediately follows that

$$E'(G) = \frac{2}{\pi} \int_0^{\infty} \ln \left| \sum_{k=0}^{n-1} c_k \, (ix)^{-k} \right| dx \, .$$

Thus, the quantity $E'(G)$ can be calculated from the coefficients of the characteristic polynomial of the graph G.

The difference $E(G) - E'(G)$ can be understood as the effect of a single zero eigenvalue, i.e., nullity $\eta = 1$, on the energy of a non-singular graph G.

Using the Coulson–Jacobs formula [11,12], we get

$$E(G) - E'(G) = Re\left[\frac{2}{\pi}\int_0^\infty \ln \frac{\sum_{k=0}^{n} c_k\,(ix)^{n-k}}{\sum_{k=0}^{n-1} c_k\,(ix)^{n-k}}\,dx\right] = \frac{2}{\pi}\int_0^\infty \ln\left|\frac{\sum_{k=0}^{n} c_k\,(ix)^{n-k}}{\sum_{k=0}^{n-1} c_k\,(ix)^{n-k}}\right| dx,$$

i.e.,

$$E(G) - E'(G) = \frac{2}{\pi}\int_0^\infty \ln\left|\frac{\phi(G,ix)}{\phi(G,ix) - c_n}\right| dx. \tag{6}$$

From Equation (6) it follows that $E(G) - E'(G) > 0$, in agreement with Conjecture 1. In order to see this, note that

$$\frac{\sum_{k=0}^{n} c_k\,(ix)^{n-k}}{\sum_{k=0}^{n-1} c_k\,(ix)^{n-k}} = \frac{A(x) - i\,B(x) + (-1)^{n/2}\,c_n}{A(x) - i\,B(x)},$$

where $A(x) = \sum_{k=0}^{n/2-1} (-1)^k\,c_{2k}\,x^{n-2k}$ and $B(x) = \sum_{k=0}^{n/2-1} (-1)^k\,c_{2k+1}\,x^{n-2k+1}$. Then

$$Re\left[\frac{\sum_{k=0}^{n} c_k\,(ix)^{n-k}}{\sum_{k=0}^{n-1} c_k\,(ix)^{n-k}}\right] = \frac{A(x)^2 + B(x)^2 + (-1)^{n/2}\,c)n}{A(x)^2 + B(x)^2} = 1 + \frac{(-1)^{n/2}\,c_n\,A(x)}{A(x)^2 + B(x)^2},$$

which by relations (3) and (4) is greater than unity for all values of $x \in [0, +\infty)$. Therefore,

$$\begin{aligned} E(G) - E'(G) &= \frac{2}{\pi}\int_0^\infty \ln\left|\frac{\sum_{k=0}^{n} c_k\,(ix)^{n-k}}{\sum_{k=0}^{n-1} c_k\,(ix)^{n-k}}\right| dx \geq \frac{2}{\pi}\int_0^\infty \ln Re\left[\frac{\sum_{k=0}^{n} c_k\,(ix)^{n-k}}{\sum_{k=0}^{n-1} c_k\,(ix)^{n-k}}\right] dx \\ &= \frac{2}{\pi}\int_0^\infty \ln\left[1 + \frac{(-1)^{n/2}\,c_n\,A(x)}{A(x)^2 + B(x)^2}\right] dx > 0\,. \end{aligned}$$

Formula (6) makes it possible to directly compute the effect of nullity in the special case of $\eta(G) = 0$ and $\eta(G') = 1$, using only the spectrum of the graph G. Numerical examples will be communicated at some later moment.

A same kind of consideration for the case $\eta(G) = 0$ and $\eta(G') = 2$, leads to

$$E(G) - E'(G) = \frac{2}{\pi}\int_0^\infty \ln\left|\frac{\sum_{k=0}^{n} c_k\,(ix)^{n-k}}{\sum_{k=0}^{n-2} c_k\,(ix)^{n-k}}\right| dx,$$

i.e.,

$$E(G) - E'(G) = \frac{2}{\pi}\int_0^\infty \ln\left|\frac{\phi(G,ix)}{\phi(G,ix) - c_n - c_{n-1}\,ix}\right| dx\,.$$

Other, more complicated cases can be treated in an analogous manner.

Conflicts of Interest: "The author declares no conflict of interest."

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