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Dependence of Graph Energy on Nullity: A Case Study

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Abstract

The nullity n_0 of a graph G is the algebraic multiplicity of the number zero in the spectrum of G. The energy $\mathcal{E}$ of G is the sum of absolute values of the eigenvalues of G. A long–open problem in the theory of graph energy is the relation between $\mathcal{E}$ and n_0, i.e., the dependence of $\mathcal{E}$ on n_0. Arguments from quantum chemistry suggest that $\mathcal{E}$ should be a decreasing function of n_0, but no mathematical verification of this conjecture is known. We now offer a case study, in which the validity of the conjecture is confirmed within a special class of graphs called banana trees.

1 Introduction

Let G be a simple graph of order n and let $\mathbf{A}(G)$ be its adjacency matrix. The eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ of $\mathbf{A}(G)$ are referred to as the eigenvalues of the graph G and form the spectrum of G [2,3].

The multiplicity of the number zero in the spectrum of G is the *nullity* of G and will be denoted by $n_0 = n_0(G)$. The sum of absolute values of the eigenvalues of G, i.e.,

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

is the *energy* of G. Both n_0 and $\mathcal{E}$ have been extensively studied within spectral graph theory, for details and further references see [7, 12, 14].

In chemical applications, when G is a graph representation of a conjugated hydrocarbon, $\mathcal{E}(G)$ is related to the total energy of the π-electrons of this hydrocarbon whereas n_0 is the number of so-called non-bonding molecular orbitals (NBMOs); for details see [4–6]. The NBMOs pertain to π-electrons which do not contribute to the chemical bonding in the underlying molecule. In view of this, from a quantum–chemical point of view, the greater is n_0, the weaker should be the bonding in the molecule and, consequently, the smaller should $\mathcal{E}$ be. In mathematical language, the parameter n_0 is expected to have a diminishing effect on the value of $\mathcal{E}$.

The above conjectured property of graph energy is not easy to formulate in a satisfactorily consistent manner. Its naive statement could be

$$n_0(G_1) > n_0(G_2) \quad \Longrightarrow \quad E(G_1) < E(G_2) \tag{2}$$

where it must be assumed that all other structural features of the graphs G_1 and G_2, influencing the value of their energies, are same or differ negligibly.

Much work has been devoted to the analysis of the dependence of $\mathcal{E}(G)$ on the structure of the graph G [6, 12]. This dependence is known to be complex, with various structural features influencing the $\mathcal{E}$-value simultaneously and in a mutually interlaced manner.

Anyway, the main structural details on which the $\mathcal{E}$-value depends are the number of vertices, number of edges, and the number, type and mutual arrangement of cycles. Thus, in order that the conjectured relation (2) be meaningful, these must be kept equal in G_1 and G_2. The elements of the set $\mathcal{B}(n)$, defined in the subsequent section, satisfy these requirements.

In an earlier work [8], the validity of the conjecture (2) was corroborated, and the n_0-dependence of $\mathcal{E}$ quantitatively assessed, by means of computer-aided numerical calculations, as applied to a suitably constructed class of graphs. In the present work we offer a model, within which the analysis of the n_0-dependence of $\mathcal{E}$ can be achieved in an explicit and mathematically exact manner.

2 Banana trees

The k-star is the tree with k vertices and $k-1$ leaves (= pendent vertices). The *banana tree*, denoted by $B(p,k)$, with parameters $p \geq 1$ and $k \geq 3$ is obtained from p disjoint k-stars, by connecting one leaf of each k-star with a single vertex that is distinct from all stars. Thus $B(p,k)$ has

$$n = n(B(p,k)) = pk + 1 \tag{3}$$

vertices.

Throughout this paper, it is assumed that the banana trees are constructed from mutually isomorphic star-graphs (i.e., that all their k-values are equal). If this condition would not be satisfied, then we would arrive at expressions much more complicated than the present Eqs. (9) and (10). Then the analytical treatment of the nullity–dependence of graph energy (as in Section 4) would not be feasible.

The parameter k is required to be at least 3. The case of $k = 1$ is formally impossible because the 1-star has no pendent vertices. In the case of $k = 2$, the banana tree would coincide with the "sun graph" of degree p (see [9]) whose nullity is equal to one, independently of the value of the parameter p. Thus, in this case, Eq. (4) would not hold.

The set of all banana trees of order n will be denoted by $\mathcal{B}(n)$. The number of elements of $\mathcal{B}(n)$ is equal to the number of solutions of the Diophantine equation $p\,k = n-1$ for $p \geq 1$ and $k \geq 3$. Thus, if $n-1$ is prime, then $\mathcal{B}(n)$ has just a single element, with $p = 1$. If $n-1$ is two times a prime, then $|\mathcal{B}(n)| = 2$, for $p = 1$ and $p = 2$. If $n-1$ is eight times a prime, then $|\mathcal{B}(n)| = 6$ for $p = 1$, $p = 2$, $p = 4$, $p = 8$, $p = (n-1)/4$, and $p = (n-1)/8$.

Properties of banana trees of have been studied in numerous earlier works (see e.g. [1, 10, 11, 13]).

As shown in the subsequent section, the nullity of $B(p,k)$ is equal to

$$n_0 = n_0(B(p,k)) = p(k-2) - 1\,. \tag{4}$$

From Eq. (3) we see that for a given value n, the set $\mathcal{B}(n)$ may consist of several banana trees. According to Eq. (4), these banana trees will have different nullities. An example is given in the following table, for the six distinct elements of $\mathcal{B}(25)$.

p	k	n_0
1	24	21
2	12	19
3	8	17
4	6	15
6	4	11
8	3	7

Combining Eqs. (3) and (4), we get $n_0 = n - 2p - 2$. Since $p \geq 1$, we thus see that

$$n_0 \leq n - 4\,. \tag{5}$$

3 Energy and Nullity of Banana Trees

The energy of a banana tree $B(p,k)$ can be determined in the standard way:
1. Calculate the characteristic polynomial of $B(p,k)$. From it, the nullity of $B(p,k)$ will be immediately seen.
2. Find the zeros of the characteristic polynomial (i.e., the graph eigenvalues)
3. Find the expression for energy using Eq. (1).

The following result is well known.

Lemma 1. [2] *Let u be a vertex of a tree T, adjacent to the vertices $v_1, v_2, \ldots, v_p$. Let $\phi(T,\lambda)$ be the characteristic polynomial of T. Then,*

$$\phi(T,\lambda) = \lambda\,\phi(T\backslash u,\lambda) - \sum_{i=1}^{p} \phi(T\backslash\{u,v_i\},\lambda).$$

Proposition 2. *The characteristic polynomial of the banana tree $B(p,k)$ is*

$$\phi(B(p,k),\lambda) = \lambda^{p(k-2)-1}\big[\lambda^2 - (k-1)\big]^{p-1}\big[\lambda^4 - (p+k-1)\lambda^2 - (k-2)p\big]\,. \tag{6}$$

Proof. Let u be the vertex of $B(p,k)$ that is distinct from all stars. If we remove u from $B(p,k)$ the subgraph $B(p,k)\backslash u$ consists of p disjoint copies of k-stars. Since the characteristic polynomial of the disjoint union of graphs is the product of their characteristic polynomials, and since the characteristic polynomial of the k-star is $\lambda^k - (k-1)\,\lambda^{k-2}$,

$$\phi(B(p,k)\backslash u, \lambda) = \left[\lambda^k - (k-1)\,\lambda^{k-2}\right]^p = \lambda^{p(k-2)}\left[\lambda^2 - (k-1)\right]^p . \tag{7}$$

The subgraph $B(p,k)\backslash\{u,v\}$, where v is a leaf of a k-star, consists of $p-1$ disjoint copies of k-stars and a $(k-1)$-star. Thus,

$$\phi(B(p,k)\backslash\{u,v\}) = \left[\lambda^k - (k-1)\,\lambda^{k-2}\right]^{p-1}\left[\lambda^{k-1} - (k-2)\,\lambda^{k-3}\right]$$

and

$$\sum_{i=1}^{p} \phi(B(p,k)\backslash\{u,v_i\},\lambda) = p\Big\{\left[\lambda^k - (k-1)\,\lambda^{k-2}\right]^{p-1}\left[\lambda^{k-1} - (k-2)\,\lambda^{k-3}\right]\Big\}. \tag{8}$$

By Lemma 1,

$$\phi(B(p,k),\lambda) = \lambda\,\phi(B(p,k)\backslash u,\lambda) - \sum_{i=1}^{p}\phi(B(p,k)\backslash\{u,v_i\},\lambda)$$

which combined with Eqs. (7) and (8) yields formula (6). □

Directly from Eq. (6) follows:

Theorem 1. *The nullity of the banana tree $B(p,k)$ is equal to $p(k-2)-1$, i.e., Eq. (4) holds.*

Proposition 3. *The energy of the banana tree $B(p,k)$ is*

$$\mathcal{E}(B(p,k)) = 2(p-1)\sqrt{k-1} + 2\sqrt{\left(\sqrt{k-2}+\sqrt{p}\right)^2 + 1}\,. \tag{9}$$

Proof. The zeros of the polynomial (6), i.e., the eigenvalues of $B(p,k)$ are:

0	$p(k-2)-1$	times
$+\sqrt{k-1}$	$p-1$	times
$-\sqrt{k-1}$	$p-1$	times

as well as the four numbers

$$\pm\sqrt{\frac{1}{2}\left[p+k-1\pm\sqrt{(p+k-1)^2-4p(k-2)}\right]}\,.$$

Substituting these into Eq. (1), and performing appropriate algebraic transformations results in formula (9). □

From Eqs. (3) and (4) we can express the parameters p and k as:

$$p=\frac{n-2-n_0}{2} \qquad \text{and} \qquad k=\frac{2(n-1)}{n-2-n_0}\,.$$

When these expressions are substituted into Eq. (9), we get an explicit functional dependence of the energy on nullity.

Theorem 2. *The energy and the nullity of a banana tree $B\in\mathcal{B}(n)$ are related as:*

$$\begin{aligned}\mathcal{E}(B) &= (n-4-n_0)\sqrt{\frac{2(n-1)}{n-2-n_0}-1}\\ &+ 2\sqrt{\left(\sqrt{\frac{2(n-1)}{n-2-n_0}-2}+\sqrt{\frac{n-2-n_0}{2}}\right)^2+1}\,. \end{aligned} \tag{10}$$

Note that Eq. (10) appears to be be the very first exact analytical expression for the dependence of graph energy on nullity. Recall that by (5), $0\le n_0\le n-4$.

Now, the task would be to prove that the function

$$f(x)=(n-4-x)\sqrt{\frac{2(n-1)}{n-2-x}-1}\;+\;2\sqrt{\left(\sqrt{\frac{2(n-1)}{n-2-x}-2}+\sqrt{\frac{n-2-x}{2}}\right)^2+1} \tag{11}$$

is monotonically decreasing for $x\in(0,n-4)$. This we verify in the subsequent section.

4 Dependence of Energy on Nullity

Theorem 3. *For a fixed number of vertices n, the energies of the banana trees $B\in\mathcal{B}(n)$ decrease as their nullities n_0 increase.*

Proof. Let n be a constant and $x \in (0, n-4)$. If we consider the function (11), then

$$f'(x) = -\frac{x+2}{\sqrt{n-x-2}\sqrt{n+x}} - \frac{\sqrt{n+x}}{(n-x-2)^{3/2}} + \frac{2\,F_0(n,x)\,F_1(n,x)}{F_2(n,x)}\,.$$

where

$$\begin{aligned}
F_0(n,x) &:= \sqrt{\frac{2(n-1)}{n-x-2}-2} + \sqrt{\frac{n-x-2}{2}} \\
F_1(n,x) &:= \frac{n-1}{\sqrt{\frac{2(n-1)}{n-x-2}-2}\,(n-x-2)^2} - \frac{1}{2\sqrt{2}\sqrt{n-x-2}} \\
F_2(n,x) &:= \sqrt{\left(\sqrt{\frac{2(n-1)}{n-x-2}-2} + \sqrt{\frac{n-x-2}{2}}\right)^2 + 1}\,.
\end{aligned}$$

If $F_1(n,x) < 0$, then $f'(x) < 0$ and the function is monotonically decreasing for $x \in (0, n-4)$. In the case when $F_1(n,x) > 0$, since $F_2(n,x) > F_0(n,x)$, we have

$$\frac{2\,F_0(n,x)\,F_1(n,x)}{F_2(n,x)} < 2\,F_1(n,x)\,.$$

Thus,

$$\begin{aligned}
f'(x) &< -\frac{x+2}{\sqrt{n-x-2}\sqrt{n+x}} - \frac{\sqrt{n+x}}{(n-x-2)^{3/2}} + \frac{2}{\sqrt{n-x-2}\sqrt{2x+2}} \\
&+ \frac{\sqrt{2x+2}}{(n-x-2)^{3/2}} - \frac{1}{\sqrt{2}\sqrt{n-x-2}}\,.
\end{aligned}$$

By direct checking it can be verified that the above inequality holds for $x = 0, 1, 2$. Therefore, it remains to consider the case $3 \le x \le n-4$. Since

$$\sqrt{n+x} \ge \sqrt{2x+4} > \sqrt{2x+2}$$

it follows

$$-\frac{\sqrt{n+x}}{(n-x-2)^{3/2}} + \frac{\sqrt{2x+2}}{(n-x-2)^{3/2}} < 0\,.$$

Also, for $x \ge 3$,

$$-\frac{1}{\sqrt{2}\sqrt{n-x-2}} + \frac{2}{\sqrt{n-x-2}\sqrt{2x+2}} < 0\,.$$

Thus $f'(x) < 0$, and Theorem 3 follows. □

Corollary 4. *In the class $\mathcal{B}(n)$ of banana trees with a fixed number of vertices n, the banana trees $B(1, n-1)$ has the minimum energy.*

It is worth noting that $B(1, n-1)$ happens to be the tree of order n with second–minimal energy.

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