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Energy, Hosoya index and Merrifield–Simmons index of trees with prescribed degree sequence[☆]

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ABSTRACT

The energy of a graph, defined as the sum of the absolute values of its eigenvalues, the number of independent edge subsets (known as Hosoya index) and the number of independent vertex subsets (called Merrifield–Simmons index) are three closely related graph invariants that are studied in mathematical chemistry. In this paper, we characterize the unique (up to isomorphism) tree which has a given degree sequence, minimum energy and Hosoya index and maximum Merrifield–Simmons index. We also compare different degree sequences and show how various known results follow as simple corollaries from our main theorem.

1. Introduction

Let G be a simple graph. The Merrifield–Simmons index $\sigma(G)$ of G is defined as the number of independent vertex subsets of G, including the empty set. Let $\mathrm{m}(G, k)$ denote the number of independent edge subsets of order k in G. The Hosoya index $\mathrm{Z}(G)$ is defined as the total number of matchings in G, i.e.,

$$\mathrm{Z}(G) = \sum_{k\geq 0} \mathrm{m}(G, k). \tag{1}$$

It is well-known that for any tree T whose adjacency matrix is $A(T)$, the sum of the absolute values of the eigenvalues of $A(T)$, which is called the energy of T and denoted by $\mathrm{En}(T)$, satisfies the relation [10]

$$\mathrm{En}(T) = \frac{2}{\pi}\int_0^\infty \frac{dx}{x^2} \log \sum_{k\geq 0} \mathrm{m}(G, k)x^{2k}. \tag{2}$$

En, Z and σ are among the most popular graph invariants that have applications in chemistry. They are used to predict, from the structure of molecules, some of their physico-chemical properties such as boiling points and π-electron energy [5,7,11]. Combined with purely mathematical interest, this has motivated intensive studies of these three graph invariants leading to a rich literature.

Most of the work deals with the characterization of the extremal graphs with respect to one or more of the three invariants in a specific class. For two disjoint graphs G and G' it is easy to see that $\sigma(G \cup G') = \sigma(G)\sigma(G')$, $\mathrm{Z}(G \cup G') = \mathrm{Z}(G)\mathrm{Z}(G')$

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and $\mathrm{En}(G \cup G') = \mathrm{En}(G) + \mathrm{En}(G')$. In view of these relations, most authors only study connected graphs. One of the most thoroughly studied classes is that of trees [16,23,18,6,15,1,8,17,24,13,14,2], its elements are connected graphs with least number of edges and hence less complicated structure. Extremal n-vertex trees with respect to each of the three invariants are path and star; see [10,18,6]. Further conditions on the number of leaves [17,24], diameter [16,23] or degrees [13,14,2] can also be imposed. In particular, the main result of [14,2] is a characterization of the n-vertex tree whose maximum degree is $d+1$, which has maximum Merrifield–Simmons index and minimum energy and Hosoya index, for all positive integers n and d. The class $\mathbb{T}_{1,d}$ of trees whose degrees are either 1 or $d \geq 2$, is studied in [13]. The two trees in $\mathbb{T}_{1,d}$ with largest Hosoya index and energy and smallest Merrifield–Simmons index are characterized for any possible number of vertices. The interested reader is referred to the surveys [9] for the energy and [20] for the Hosoya index and Merrifield–Simmons index.

For all trees of order n whose vertex degrees are $d_1 \geq \cdots \geq d_n$, the n-tuple $(d_1, \ldots, d_n)$ is called degree sequence of T. Pursuing the work in [13,14,2], it is natural to consider the class $\mathbb{T}(D)$ of all trees which has a given degree sequence D. Trees with prescribed degree sequence have also been studied in the context of other graphs invariants, such as the spectral radius [25,3] and Wiener-type graph invariants [19,21,22]. In this paper we investigate the energy, Hosoya index and Merrifield–Simmons index of trees in $\mathbb{T}(D)$, for arbitrary D. We find that for any degree sequence D, there exists a tree $\mathcal{M}(D) \in \mathbb{T}(D)$ such that whenever $T \in \mathbb{T}(D)$ either T and $\mathcal{M}(D)$ are isomorphic or the three inequalities $\mathrm{En}(\mathcal{M}(D)) < \mathrm{En}(T)$, $\mathrm{Z}(\mathcal{M}(D)) < \mathrm{Z}(T)$ and $\sigma(\mathcal{M}(D)) > \sigma(T)$ hold. Sections 2–4 are devoted to proving this observation and to describing the construction of $\mathcal{M}(D)$. As an additional result we show in Section 5 that if $B = (b_1, \ldots, b_n)$ and $D = (d_1, \ldots, d_n)$ are two different degree sequences such that

$$\sum_{i=1}^{k} b_i \leq \sum_{i=1}^{k} d_i$$

for all $1 \leq k \leq n$, then we have $\sigma(\mathcal{M}(B)) < \sigma(\mathcal{M}(D))$, $\mathrm{Z}(\mathcal{M}(B)) > \mathrm{Z}(\mathcal{M}(D))$ and $\mathrm{En}(\mathcal{M}(B)) > \mathrm{En}(\mathcal{M}(D))$. Several older results, which follow directly from this, will be revisited as applications of our main theorem.

We reduce the study of En and Z to that of an auxiliary invariant defined for all trees T and real $x > 0$ by

$$\mathrm{M}(T, x) = \sum_{k \geq 0} \mathrm{m}(T, k) x^k,$$

since (1) and (2) can be rewritten as

$$\mathrm{Z}(T) = \mathrm{M}(T, 1) \tag{3}$$

and

$$\mathrm{En}(T) = \frac{2}{\pi} \int_0^\infty \frac{dx}{x^2} \log \sum_{k \geq 0} \mathrm{M}(T, x^2), \tag{4}$$

respectively.

For undefined notations and terminology, the reader is referred to [4].

2. Preliminaries

Definition 1. If $(d_1, \ldots, d_n, 1, \ldots, 1)$ is the degree sequence of a tree T, where $d_n \geq 2$, then we call the n-tuple $(d_1, \ldots, d_n)$ *reduced degree sequence* of T.

For every tree with reduced degree sequence $(d_1, \ldots, d_n)$ and k leaves, the Handshake lemma gives $k + \sum_{j=1}^{n} d_j = 2(n-1)$. This shows that two trees with the same reduced degree sequence have the same number of leaves, hence they have the same degree sequence.

Definition 2. We call a subgraph B of a tree T a *complete branch* of T if and only if T can be decomposed as in Fig. 1(a), where B and $T - B$ are non-empty.

For example, if T is the tree in Fig. 1(b), then the subgraph spanned by $\{v_1, v_2, v_3, v_4\}$ is a complete branch, but the subgraph spanned by $\{v_1, v_2, v_4\}$ is not. For any complete branch B of T, we define its root to be the unique vertex which has a neighbour in $T - B$. We will denote by $\mathrm{r}(B)$ the root of B, $\mathrm{rn}(B)$ its neighbour in $T - B$, and $\mathrm{rd}(B)$ the degree of $\mathrm{r}(B)$ as a vertex of B. If $B_1, \ldots, B_{\mathrm{rd}(B)}$ are the connected components of $B - \mathrm{r}(B)$, then we write $B = [B_1, \ldots, B_{\mathrm{rd}(B)}]$.

For any two rooted trees R and R', we write $R \approx_r R'$ if and only if there exists an isomorphism $R \to R'$ which preserves the roots, otherwise we write $R \not\approx_r R'$.

Definition 3. We call a vertex in a tree a *pseudo-leaf* if and only if it is not a leaf and it has at most one neighbour with degree greater than 1. We call a complete branch whose root is a pseudo-leaf a *pseudo-leaf branch*.

We denote by $[d]$ a pseudo-leaf branch with d vertices.