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Research Article

Comparing degree–based energies of trees

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Abstract

A Coulson-type integral formula for the degree-based energies of trees is established. Based on it, the energies pertaining to various degree-based invariants of trees are compared, and also they are compared with the ordinary energy.

Keywords: energy (of graph); degree (of vertex); degree-based topological index.

2020 Mathematics Subject Classification: 05C50, 05C03, 05C07, 05C31.

1. Introduction

In this paper we are concerned with trees and their degree-based energies. Let G be a simple graph, with vertex set $\mathbf{V}(G)$ and edge set $\mathbf{E}(G)$. Then $|\mathbf{V}(G)|$ and $|\mathbf{E}(G)|$ are, respectively, the number of vertices and edges of G. Let $|\mathbf{V}(G)| = n$.

By $uv \in \mathbf{E}(G)$ we denote the edge of G, connecting the vertices u and v. The degree (= number of first neighbors) of a vertex $u \in \mathbf{V}(G)$ is denoted by $d(u)$.

By definition, a tree T is a connected simple graph with n vertices and $n-1$ edges. Alternatively, a tree is defined as a connected graph without cycles.

For other graph-theoretical notions, the readers are referred to textbooks [2, 28].

In the mathematical and chemical literature, several dozens of vertex–degree–based graph invariants, usually referred to as "topological indices" (TIs), have been and are currently studied [26, 27]. Most of these are of the form

$$TI(G) = \sum_{uv\in\mathbf{E}(G)} F_{TI}\big(d(u), d(v)\big) \tag{1}$$

where $F_{TI}(x,y)$ is an appropriately chosen function with the property $F_{TI}(x,y) = F_{TI}(y,x)$. Since the variables in $F_{TI}(x,y)$ are vertex degrees, they are integers, satisfying $x \geq 1$ and $y \geq 1$. In all hitherto proposed topological indices of the form (1) (cf. [12, 26, 27]), the function $F_{TI}(x,y)$ has non-negative values for all $x, y \geq 1$.

The oldest among such graph invariants, conceived as early as in the 1970s, are the first and second Zagreb indices, Zg_1 and Zg_2 [15, 16]. Their F-functions are

$$F_{Zg_1}(x,y) = x + y \tag{2}$$

and

$$F_{Zg_2}(x,y) = x\,y\,. \tag{3}$$

Some other topological indices of this kind, to be examined in the later parts of this paper, are the Randić connectivity index R [23], the atom-bond connectivity index ABC [7], the sum-connectivity index SCI [29], the Sombor index SO [12], and the Nirmala index Ni [19]. Their F-functions are

$$F_R(x,y) = \frac{1}{\sqrt{x\,y}} \tag{4}$$

$$F_{ABC}(x,y) = \sqrt{\frac{x+y-2}{x\,y}} \tag{5}$$

$$F_{SCI}(x,y) = \frac{1}{\sqrt{x+y}} \tag{6}$$

$$F_{SO}(x,y) = \sqrt{x^2+y^2} \tag{7}$$

$$F_{Ni}(x,y) = \sqrt{x+y}\,. \tag{8}$$

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The vertices of the graph G will be labeled by $1,2,\dots,n$. Then the adjacency matrix of G, denoted by $\mathbf{A}(G)$, is defined as the symmetric square matrix of order n, whose (i,j)-element is

$$\mathbf{A}(G)_{ij} = \begin{cases} 1 & \text{if } ij \in \mathbf{E}(G) \\ 0 & \text{if } ij \notin \mathbf{E}(G) \\ 0 & \text{if } i = j\,. \end{cases}$$

The eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_n$ of $\mathbf{A}(G)$ form the spectrum of the graph G. The characteristic polynomial of $\mathbf{A}(G)$ is defined as

$$\phi(G,\lambda) = \det\big(\lambda\,\mathbf{I}_n - \mathbf{A}(G)\big) \tag{9}$$

where $\mathbf{I}_n$ is the unit matrix of order n. Recall that λ_i , $i = 1,2,\dots,n$, are the zeros of $\phi(G,\lambda)$, i.e., satisfy the condition $\phi(G,\lambda_i) = 0$.

The energy of the graph G is defined as [20]

$$En(G) = \sum_{i=1}^{n} |\lambda_i|\,. \tag{10}$$

This graph invariant was put forward in the 1970s, motivated by the study of total π-electron energy in theoretical chemistry [13]. Since then, it became a popular topic of research, with over one thousand published papers, see [14, 20], the recent works [1, 3, 8, 18] and the references cited therein.

For more details of spectral graph theory and on graph energy see [5, 20].

Some time ago [6, 17], it was attempted to combine the theory of graph energy with the theory of vertex-degree-based topological indices. For this, using formula (1), an adjacency–matrix–type square symmetric matrix $\mathbf{A}_{TI}(G)$ was introduced, whose (i,j)-element is

$$\mathbf{A}_{TI}(G)_{ij} = \begin{cases} F_{TI}\big(d(i),d(j)\big) & \text{if } ij \in \mathbf{E}(G) \\ 0 & \text{if } ij \notin \mathbf{E}(G) \\ 0 & \text{if } i = j\,. \end{cases}$$

The theory based on the matrix $\mathbf{A}_{TI}$ and its spectrum was recently elaborated in some detail [21, 25].

The eigenvalues of $\mathbf{A}_{TI}(G)$ will be denoted by $\theta_1, \theta_2, \dots, \theta_n$, and are said to form the *TI-spectrum* of the graph G. The *TI-characteristic polynomial* is defined as

$$\phi_{TI}(G,\lambda) = \det\big(\lambda\,\mathbf{I}_n - \mathbf{A}_{TI}(G)\big)$$

in analogy to Equation (9). Thus θ_i , $i = 1,2,\dots,n$, are the zeros of $\phi_{TI}(G,\lambda)$, i.e., satisfy the condition $\phi_{TI}(G,\theta_i) = 0$. In analogy to Equation (10), it was found purposeful to define the *TI-energy* as [6]

$$En_{TI}(G) = \sum_{i=1}^{n} |\theta_i|\,. \tag{11}$$

Remark 1.1. *All edges of the n-vertex star S_n connect vertices of degree 1 and $n-1$. Therefore, for any vertex–degree–based topological index TI satisfying Equation (1),*

$$\mathbf{A}_{TI}(S_n) = F_{TI}(1,n-1)\,\mathbf{A}(S_n)$$

implying $\theta_i = F_{TI}(1,n-1)\,\lambda_i$ for $i = 1,2,\dots,n$, and

$$En_{TI}(S_n) = F_{TI}(1,n-1)\,En(S_n) = 2\sqrt{n-1}\,F_{TI}(1,n-1)\,.$$

2. The TI-energy of a tree

In what follows, we focus our attention to trees. Let T be a tree on n vertices, $n \geq 2$. The main result in the spectral theory of trees is the formula [5, 9, 10, 28]

$$\phi(T,\lambda) = \lambda^n + \sum_{k\geq 1} (-1)^k\, m(T,k)\, \lambda^{n-2k} \tag{12}$$

where $m(T,k)$ stands for the number of k-matchings (= selections of k mutually independent edges) in the tree T. By definition, $m(T,1) = n-1$.

The matrix $\mathbf{A}_{TI}(G)$ can be viewed as the adjacency matrix of a graph with weighted edges, the weight of the edge uv being $F_{TI}\big(d(u),d(v)\big)$. This, of course, applies also to trees.

According to the Sachs coefficient theorem [5,24], for the TI-characteristic polynomial of a tree T, an expression analogous to Equation (12) would hold, namely

$$\phi_{TI}(T,\lambda) = \lambda^n + \sum_{k\geq 1} (-1)^k \, m_{TI}(T,k) \, \lambda^{n-2k} \,. \tag{13}$$

The coefficient $m_{TI}(T,k)$ is equal to the sum of weights coming from all k-matchings of T. Each particular k-matching contributes to $m_{TI}(T,k)$ by the product of the squares of the terms $F_{TI}\big(d(u),d(v)\big)$, pertaining to the edges contained in that matching [24]. Thus, let M be a distinct k-matching of T, and let $\mathcal{M}(k)$ be the set of all such k-matchings. Then for $k \geq 1$, $\mathcal{M}(k)$ consists of $m(T,k)$ elements, i.e., $|\mathcal{M}(k)| = m(T,k)$.

The weight of a single matching M is equal to

$$\prod_{uv\in M} \left[F_{TI}\big(d(u),d(v)\big)\right]^2$$

and therefore

$$m_{TI}(T,k) = \sum_{M\in\mathcal{M}(k)} \prod_{uv\in M} \left[F_{TI}\big(d(u),d(v)\big)\right]^2 \tag{14}$$

provided $\mathcal{M}(k) \neq \emptyset$. If, on the other hand, $\mathcal{M}(k) = \emptyset$, then $m_{TI}(T,k) = 0$.

The fact that the energy of a graph can be directly computed from the characteristic polynomial (without knowing the graph eigenvalues, i.e., without using Equation (10)) was discovered by Coulson in 1940 [4]. In that time, formula (12) was not known. Much later, the following Coulson-type integral formula was obtained for the energy of trees [11]:

$$En(T) = \frac{2}{\pi} \int\limits_0^\infty \frac{dx}{x^2} \ln \left[1 + \sum_{k\geq 1} m(T,k)\, x^{2k}\right] dx \,. \tag{15}$$

The analogous expression for the TI-energy is

$$En_{TI}(T) = \frac{2}{\pi} \int\limits_0^\infty \frac{dx}{x^2} \ln \left[1 + \sum_{k\geq 1} m_{TI}(T,k)\, x^{2k}\right] dx \tag{16}$$

and can be obtained in the exactly same manner as Equation (15) [11,22]. What is most important is that the coefficients $m_{TI}(T,k)$ are non-negative, and that the TI-energy is a monotonically increasing function of these coefficients.

From a formal point of view, Equations (15) and (16) appear to be fully analogous. However, from Equations (13) and (14) we see that the structure-dependency of the TI-characteristic polynomial (i.e., of its coefficients) is perplexed, and by no means easy to comprehend. The same conclusion applies to formula (16). Yet, we can use (15) and (16) to compare TI-energies of various topological indices. These results are collected in the subsequent section.

3. Comparing TI-energies of trees

Theorem 3.1. *Let TI_a and TI_b be two degree–based topological indices, defined according to formula (1). Let T be any tree. If $F_{TI_a}(x,y) \geq F_{TI_b}(x,y)$ holds for all $x,y \geq 1$, then $En_{TI_a}(T) \geq En_{TI_b}(T)$. If for a particular tree T_0, $F_{TI_a}(x_0,y_0) > F_{TI_b}(x_0,y_0)$ holds for at least one pair x_0,y_0, then $En_{TI_a}(T_0) > En_{TI_b}(T_0)$.*

Proof. By Equation (14), the condition $F_{TI_a}(x,y) \geq F_{TI_b}(x,y)$ implies $m_{TI_a}(T,k) \geq m_{TI_b}(T,k)$ for all $k \geq 1$. Also, the condition $F_{TI_a}(x_0,y_0) > F_{TI_b}(x_0,y_0)$ implies $m_{TI_a}(T,k) > m_{TI_b}(T,k)$ for all values of k for which there exist k-matchings in the tree T_0, containing the edge x_0y_0. Theorem 3.1 follows then from formula (16). □

Theorem 3.2. *Let TI be a degree–based topological index, defined according to formula (1). Let T be any tree.*

(a) *If $F_{TI}(x,y) \geq 1$ holds for all $x,y \geq 1$, then $En_{TI}(T) \geq En(T)$. If for a particular tree T_0, $F_{TI}(x_0,y_0) > 1$ holds for at least one pair x_0,y_0, then $En_{TI}(T_0) > En(T_0)$.*

(b) *If $F_{TI}(x,y) \leq 1$ holds for all $x,y \geq 1$, then $En_{TI}(T) \leq En(T)$. If for a particular tree T_0, $F_{TI}(x_0,y_0) < 1$ holds for at least one pair x_0,y_0, then $En_{TI}(T_0) < En(T_0)$.*

Proof. The right–hand side of Equation (14) reduces to $m(T,k)$ if $F_{TI}(x,y) = 1$ for all $xy \in \mathbf{E}(T)$. If so, then the right–hand sides of (15) and (16) coincide. □

Applying Theorems 3.1 and 3.2 to the above listed degree–based topological indices, Equations (2)–(8), we obtain the following inequalities.

Corollary 3.1. *For $TI = Zg_1, Zg_2, SO, Ni$, and for any tree T,*

$$En_{TI}(T) > En(T)\,.$$

For $TI = R, ABC, SCI$, and for any tree T,

$$En_{TI}(T) < En(T)\,.$$

Exceptionally, if $n = 2$, i.e., if $T \cong S_2$, then $En_{Zg_2}(T) = En_R(T) = En(T) = 2$.

Proof. The inequalities stated in Corollary 3.1 follow from Equations (2)–(8), from which the conditions $TI > 1$ or $TI < 1$ are obvious. Here we only verify the relation $TI < 1$ for the ABC index, Equation (5).

For $x = 1$, $F_{ABC}(x, y) = \sqrt{(y-1)/y} < 1$. For $x = 2$, $F_{ABC}(x, y) = \sqrt{1/2} < 1$. By symmetry, the same holds for $y = 1$ and $y = 2$. What remains is to consider the case $x, y \geq 3$. This yields

$$\sqrt{\frac{x+y-2}{x\,y}} < \sqrt{\frac{x+y}{x\,y}} = \sqrt{\frac{1}{x}+\frac{1}{y}} \leq \sqrt{\frac{1}{3}+\frac{1}{3}} = \sqrt{\frac{2}{3}} < 1\,.$$

□

Bearing in mind the evident relations

$$x + y > \sqrt{x^2+y^2} > \sqrt{x+y} \qquad \text{and} \qquad \frac{1}{x\,y} < \frac{x+y-2}{x\,y}$$

we arrive at:

Corollary 3.2. *For any tree T,*

$$En_{Zg_1}(T) > En_{SO}(T) > En_{Ni}(T)$$

and

$$En_R(T) < En_{ABC}(T)$$

except for $T \cong S_2$, in which case $2 = En_R(S_2) > En_{ABC}(S_2) = 0$.

Remark 3.1. *The two Zagreb indices are not comparable because of*

$$F_{Zg_1}(1,3) > F_{Zg_2}(1,3) \qquad \textit{whereas} \qquad F_{Zg_1}(2,3) < F_{Zg_2}(2,3)\,.$$

The Randić and sum-connectivity indices are not comparable because of

$$F_R(1,3) > F_{SCI}(1,3) \qquad \textit{whereas} \qquad F_R(2,3) < F_{SCI}(2,3)\,.$$

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