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Counterexamples to conjectures on graph distance measures based on topological indexes

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ABSTRACT

In this paper we disprove three conjectures from Dehmer et al. (2014) on graph distance measures based on topological indices by providing explicit classes of trees that do not satisfy proposed inequalities. The constructions are based on the families of trees that have the same Wiener index, graph energy or Randić index – but different degree sequences.

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1. Introduction

The structural graph similarity or distance of graphs has been attracting attention of researchers from many different fields, such as mathematics, social network analysis, biology or chemistry. The two main concepts which have been explored are exact (based on isomorphic relations and computationally demanding, see [7,8] and references therein) and inexact graph matching (one example here is graph edit distance, see [4]). In this paper we are dealing with the later concept, and study interrelations of graph distance measures by means of inequalities. Graph distance measure is a mapping $d : \mathcal{G} \times \mathcal{G} \to R^+$, where $\mathcal{G}$ is any set of graphs [12].

Given two graphs with n vertices, G_1 and G_2, the edit distance between G_1 and G_2, denoted by $GED(G_1, G_2)$, is the minimum cost caused by the number of edge additions and/or deletions that are needed transform G_1 into G_2. GED has been introduced by Bunke [3].

A topological index [22] is a type of a molecular descriptor that is calculated based on the molecular graph of a chemical compound, and usually represents numerical graph invariant $I(G)$.

Some novel class of graph distance measures based on topological indices have been introduced by Dehmer et al. [9]. The same authors continued research from [10] and proved various inequalities and studied comparative graph measures based on the well-known Wiener index, graph energy and Randić index. For more results on graph entropy measures see [5,6].

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2. Preliminaries

We focus on the graph distance measure introduced in [9]:

$$d_I(G, H) = d(I(G), I(H)) = 1 - e^{-\left(\frac{I(G)-I(H)}{\sigma}\right)^2},$$

where σ is an arbitrary real number and $I(G)$ and $I(H)$ are certain graph invariants. Note that $d_I(G, H)$ is actually is a distance measure for real numbers, and for more mathematical properties see [10].

Let $G = (V, E)$ be a connected graph on n vertices. The distance between the vertices u and v of G is denoted by $d(u, v)$. The Wiener index is one of the oldest distance-based topological indexes [11,14], and defined as the sum of all distances between any two vertices of a graph:

$$W(G) = \sum_{u,v \in V} d(u, v).$$

Randić index [2,17,21] is suitable for measuring the extent of branching of chemical graphs, and is defined as

$$R(G) = \sum_{uv \in E} \frac{1}{\sqrt{deg(u)deg(v)}},$$

where $deg(v)$ is a degree of the vertex v.

Denote by $\lambda_1, \lambda_2, \ldots, \lambda_n$ the eigenvalues of the adjacency matrix of G. The energy of a graph is introduced by Gutman [18] equals to

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

while the distance measure based on Shannon's entropy [15] is defined as

$$Ig(G) = \log E(G) - \frac{1}{E(G)} \sum_{i=1}^{n} |\lambda_i| \log |\lambda_i|.$$

By setting $f(v_i) = deg(v_i)^k = deg_i^k$ in the Shannon entropy formula, we can also obtain the new entropy based on the degree powers [5,16], denoted by $If_k(G)$:

$$If_k(G) = \log \left(\sum_{i=1}^{n} deg_i^k \right) - \frac{1}{\sum_{i=1}^{n} deg_i^k} \sum_{i=1}^{n} deg_i^k \log deg_i^k.$$

The following three conjectures are proposed in the same paper of Dehmer et al.

Conjecture 1. *Let T and T' be any two trees with n vertices. Then, it holds*

$$d_W(T, T') \geq d_R(T, T').$$

Conjecture 2. *Let T and T' be any two trees with n vertices. Then, it holds*

$$d_E(T, T') \geq d_{Ig}(T, T').$$

Conjecture 3. *Let T and T' be any two trees with n vertices. Then, it holds*

$$d_R(T, T') \geq d_{If_1}(T, T')$$

In this note, we are going to construct a family of pairs of trees that do not satisfy Conjectures 1 and 3, and then disprove Conjecture 2 by providing specific examples of equienergetic trees from the literature. The authors from [9] verified the conjectures on all trees with small number of vertices and these counterexamples have more than 12 vertices. In Section 4, we are going to refine some results on the graph edit distance and Shannon entropy from [9] and [10].

3. Main results

By definition, the reverse inequality $d_W(T, T') < d_R(T, T')$ is equivalent to

$$1 - e^{-\left(\frac{W(T)-W(T')}{\sigma}\right)^2} < 1 - e^{-\left(\frac{R(T)-R(T')}{\sigma}\right)^2}.$$

Using the fact that e^x is a strictly increasing function, it is further equivalent to

$$|W(T) - W(T')| < |R(T) - R(T')|.$$

We are going to construct a family of tree pairs (T, T') on n vertices that have the same Wiener index and different Randić index, and thus left side of the above inequality will be 0. More examples of non-isomorphic trees having equal Wiener index are introduced by Rada in [20].

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