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On Topological Indices and Their Reciprocals

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Abstract

If $TI(G) = \sum\limits_{\gamma} F(\gamma)$ is a topological index of the graph G, then $RTI(G) = \sum\limits_{\gamma} \frac{1}{F(\gamma)}$ is the respective reciprocal index. In contemporary mathematical chemistry, a large number of pairs (TI, RTI) have been separately introduced and studied, but their mutual relations eluded attention. In this paper, we determine some basic relations between TI and RTI, and then focus our attention to the pair Wiener index – Harary index.

If G is a connected graph and $d(u,v)$ the distance between its vertices u and v, then the Wiener and Harary indices are $W = \sum\limits_{u,v} d(u,v)$ and $H = \sum\limits_{u,v} \frac{1}{d(u,v)}$, respectively. In this paper the product $W \cdot H$ is studied. The minimum value of $W \cdot H$ is determined for general connected graphs and conjectured for trees. The maximum value is discussed, based on our computer-aided findings.

1 Introduction

Let G be a (molecular) graph, and let γ be some structural feature of G. Then the majority of topological indices used in modern-day mathematical

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chemistry [15, 35] are of the form

$$TI = TI(G) = \sum_{\gamma \in G} F(\gamma)$$

for some pertinently chosen function F, with summation going over all fragments γ contained in G; for examples see the subsequent section. Then the *reciprocal* of TI is the topological index defined as

$$RTI = RTI(G) = \sum_{\gamma \in G} \frac{1}{F(\gamma)}\,.$$

Examples given in the subsequent section show that among the topological indices exiting in the current literature, there are quite a few (TI, RTI)-pairs.

In this paper, we are interested in the relations between TI and RTI, and especially in the properties of the product $TI \cdot RTI$.

2 Familiar indices and their reciprocals

In this section we list a few well known and much studied topological indices together with their (also well known and much studied) reciprocals.

Let the vertex and edge sets of the graph G be $\mathbf{V}(G)$ and $\mathbf{E}(G)$, respectively, and let the number of vertices and edges of G be $n = |\mathbf{V}(G)|$ and $m = |\mathbf{E}(G)|$, respectively. The edge connecting the vertices u and v is denoted by uv.

The degree (= number of first neighbors) of the vertex $u \in \mathbf{V}(G)$ will be denoted by d_u.

The following are some vertex-degree-based (TI, RTI)-pairs, among several others.

- First Zagreb index [9, 25] and harmonic index [28, 41]

$$Zg_1(G) = \sum_{uv \in \mathbf{E}(G)} (d_u + d_v) \quad \text{and} \quad Harm(G) = \sum_{uv \in \mathbf{E}(G)} \frac{2}{d_u + d_v}\,;$$

- sum-connectivity index [22, 42] and nirmala index [16]

$$SC(G)=\sum_{uv\in\mathbf{E}(G)}\frac{1}{\sqrt{d_u+d_v}}\quad\text{and}\quad N(G)=\sum_{uv\in\mathbf{E}(G)}\sqrt{d_u+d_v}\,;$$

- geometric-arithmetic index [36, 40] and arithmetic-geometric index [33, 34]

$$GA(G)=\sum_{uv\in\mathbf{E}(G)}\frac{2\sqrt{d_u\,d_v}}{d_u+d_v}\quad\text{and}\quad AG(G)=\sum_{uv\in\mathbf{E}(G)}\frac{d_u+d_v}{2\sqrt{d_u\,d_v}}\,;$$

- Randić index [26, 27] and reciprocal Randić index [10]

$$R(G)=\sum_{uv\in\mathbf{E}(G)}\frac{1}{\sqrt{d_u\,d_v}}\quad\text{and}\quad RR(G)=\sum_{uv\in\mathbf{E}(G)}\sqrt{d_u\,d_v}\,;$$

- inverse sum indeg index [3, 37] and redefined first Zagreb index [18]

$$ISI(G)=\sum_{uv\in\mathbf{E}(G)}\frac{d_u\,d_v}{d_u+d_v}\quad\text{and}\quad ReZg_1(G)=\sum_{uv\in\mathbf{E}(G)}\frac{d_u+d_v}{d_u\,d_v}\,;$$

- Sombor index [7] and modified Sombor index [13, 17]

$$SO(G)=\sum_{uv\in\mathbf{E}(G)}\sqrt{d_u^2+d_v^2}\quad\text{and}\quad {}^mSO(G)=\sum_{uv\in\mathbf{E}(G)}\frac{1}{\sqrt{d_u^2+d_v^2}}\,.$$

Let G be a connected graph and u, v two of its vertices. By $d(u,v)$ we denote the distance between these vertices (= length of a shortest path connecting u and v). Then the Wiener index [29, 38]

$$W=W(G)=\sum_{\{u,v\}\subseteq V(G)}d(u,v)\,. \tag{1}$$

and the Harary index [21, 39]

$$H=H(G)=\sum_{\substack{\{u,v\}\subseteq V(G)\\ u\neq v}}\frac{1}{d(u,v)}\,. \tag{2}$$

form an important distance-based (TI, RTI)-pair.

Remark. The relations between GA and AG, as well as SO and ${}^{m}SO(G)$, were examined in [6] and [11].

Remark. The reciprocal of the ISI-index, named *redefined first Zagreb index* ($ReZg_1$) was studied, calculated, and applied by great many authors [2, 4, 12, 14, 18, 20, 23, 24, 30, 32]. No one of them noticed the elementary fact [1]

$$ReZg_1(G) = \sum_{uv \in \mathbf{E}(G)} \frac{d_u + d_v}{d_u\, d_v} = n$$

i.e., that the “topological index“ $ReZg_1$ is fully independent of any structural detail of the underlying molecular graph. This bizarre detail reveals the level of competence of many of those who nowadays publish papers on topological indices and their applications.

3 General properties of (TI, RTI)-pairs

We first state an old, but not well know result of Schweitzer [31]:

Lemma 1. [31] *Let* $a_1, a_2, \ldots, a_p$ *be positive real numbers. Let* $A = \max\limits_{1 \le i \le p} a_i$ *and* $a = \min\limits_{1 \le i \le p} a_i$. *Then*

$$\left(\sum_{i=1}^{p} a_i\right)\left(\sum_{i=1}^{p} \frac{1}{a_i}\right) \ge \frac{(A+a)^2}{4aA}\, p^2\,. \tag{3}$$

Equality holds if and only if $a_1 = a_2 = \cdots = a_p$, *in which case the term* $(A+a)^2/(4aA)$ *is equal to unity.*

Recall that $(A+a)^2/(4aA) \ge 1$.

Using Schweitzer’s inequality, we immediately arrive at a lower bound for the product $TI \cdot RTI$ of any vertex-degree-based index of the form

$$TI = TI(G) = \sum_{uv \in \mathbf{E}(G)} F(d_u, d_v)\,, \tag{4}$$

assuming that $F(d_u, d_v) > 0$ holds for all $uv \in \mathbf{E}(G)$.

Theorem 1. *If TI satisfies Eq. (4), then for any graph with m edges,*

$$TI(G)\cdot RTI(G) \geq \frac{(F+f)^2}{4fF}\, m^2$$

where

$$F = \max_{uv\in \mathbf{E}(G)} F(d_u,d_v) \quad \text{and} \quad f = \min_{uv\in \mathbf{E}(G)} F(d_u,d_v)\,.$$

In the case of connected graphs, the product $TI(G)\cdot RTI(G)$ is minimal and equal to m^2 if and only if G is either regular or complete bipartite (in which case the term $(F+f)^2/(4fF)$ is equal to unity).

Proof. It is sufficient to observe that the values of $F(d_u,d_v)$ are mutually equal if and only if all edges of the underlying graph connect vertices of same degree pairs. In the case of connected graphs, this happens only at regular and complete bipartite graphs. ∎

Corollary. *Denote by S_n the star of order n. If T_n is an n-vertex tree, then the product $TI(T_n)\cdot RTI(T_n)$ is minimal and equal to $(n-1)^2$ if and only if $T_n \cong S_n$.*

The result of Theorem 1 is applicable to all vertex-degree-based topological indices listed in Section 2. Exceptionally, because of the multiplier 2 in the definition of the harmonic index, the lower bound for $Zg_1\cdot Harm$ is $2\,(F+f)^2/(4fF)\,m^2$ and the respective minimal value is $2m^2$.

Finding the maximum value for the product $TI{\cdot}RTI$ seems to be a much more difficult task. Our numerical experience (see [11] and the following section) indicates that a generally applicable solution does not exist, and that it differs from index to index.

4 An example: Wiener and Harary indices

The Wiener and Harary indices, Eqs. (1) and (2), are certainly the best known and most detailed studied distance-based topological indices. Thus, they form the most interesting distance-based (TI,RTI)-pair. Applying Schweitzer's inequality (3), we get:

Theorem 2. *Denote by K_n the complete graph of order n. Let G be a connected graph on n vertices and diameter D. Then*

$$W(G)\cdot H(G) \geq \frac{(D+1)^2}{4D}\binom{n}{2}^2 .$$

Equality holds if and only if $G \cong K_n$.

Proof. In the graph G there are $\binom{n}{2} = \frac{1}{2}n(n-1)$ vertex pairs. Because some vertices are adjacent, the minimum distance is 1. The maximum distance is D. Equality will happen only if all distances are equal, 1, i.e., if $D = 1$, i.e. if $G \cong K_n$. ∎

Corollary. *For connected graphs on n vertices, the minimum value of $W\cdot H$ is $n(n-1)/2$, attained for the complete graph.*

In the case of trees, the above equality holds if and only if $n = 2$. Therefore, if $n \geq 3$, then there must exist a tree (or trees) of order n, for which the product $W\cdot H$ is minimal.

In order to get some information on the product $W \cdot H$ of trees, we performed a few computational studies.

As a starter, we found that there is a remarkably good correlation between $W\cdot H$ and W. A characteristic example is shown in Fig. 1.

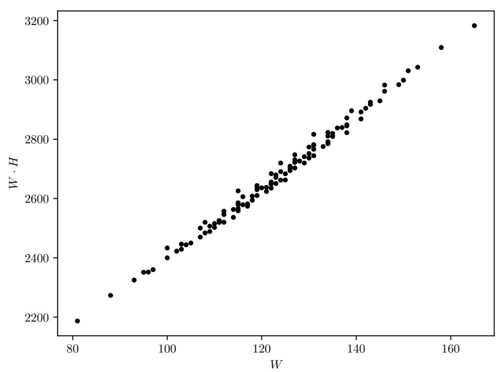

Fig. 1. Correlation between the product of Wiener and Harary indices, and the Wiener index for 10-vertex trees.

Bearing in mind the well know result that for any n-vertex tree T_n, different from the star (S_n) and the path (P_n),

$$W(S_n) < W(T_n) < W(P_n)\,,$$

from Fig. 1 one my anticipate an analogous relation for $W \cdot H$. Indeed, by checking all trees with n vertices, $4 \leq n \leq 20$, we found that the minimal and maximal values of $W \cdot H$ are attained by S_n and P_n, respectively. This encouraged us to state the following:

Conjecture 1. *Let $n \geq 5$. Let T_n be any n-vertex tree, different from the star S_n and the path P_n. Then*

$$W(S_n) \cdot H(S_n) < W(T_n) \cdot H(T_n) < W(P_n) \cdot H(P_n)\,. \tag{5}$$

What happened after this conjecture was made public, is recorded in the Editorial [8] and the paper [19]

In short: The left-hand side of (5) is generally valid, whereas for sufficiently large values of n, the right-hand side is violated.

Andrey Dobrynin [5] was the first who discovered that in the general case $W(P_n) \cdot H(P_n)$ is not maximal. In order to better understand the reasons for this violation, we determined the tree with second-maximal $W \cdot H$-value. For n up to 20, this is the snake (Sk_n), shown in Fig. 2.

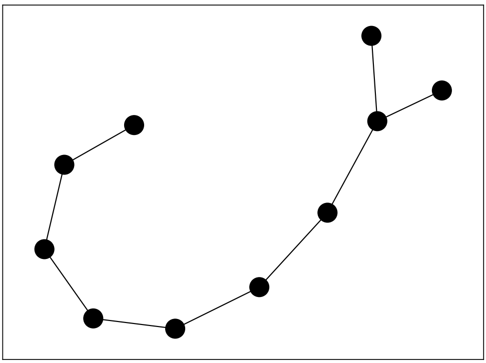

Fig. 2. The 10-vertex tree (the "snake" Sk_{10}) with second-maximal $W \cdot H$-value. Such trees are found to be second-maximal for $4 \leq n \leq 20$.

Direct calculation reveals that the relation

$$W(P_n)\cdot H(P_n) - W(Sk_n)\cdot H(Sk_n) > 0$$

holds up to $n = 37$, and that this difference changes sign at $n = 38$, see Fig. 3.

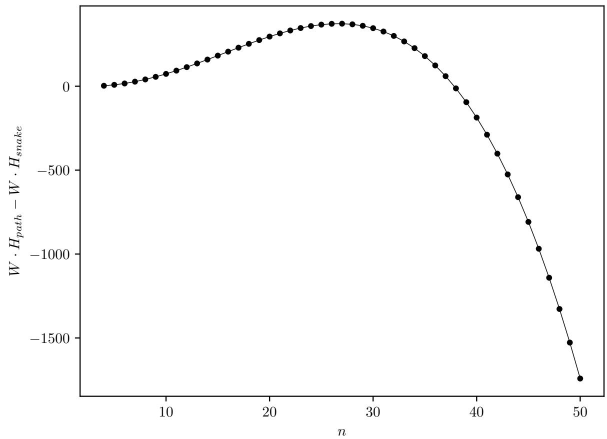

Fig. 3. The size-dependence of the difference of the product $W\cdot H$ of the path and the snake.

This indicates, that counterexamples for the right-hand side of (5) exist for all $n \geq 38$.

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