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A Note on Topological Indices and Their Reciprocals

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Abstract

We correct the inequality in Lemma 1 of "On Topological Indices and Their Reciprocals" and the resulting bounds in Theorems 1 and 2. We classify the lower-bound equality cases for all six degree-based pairs in the paper, disprove the tree corollary following Theorem 1, correct the minimum Wiener–Harary product over connected graphs, and determine the leading asymptotic term of the maximum Wiener–Harary product over trees.

In Lemma 1 of [1], the inequality has the wrong direction; the quantities printed as lower bounds in Theorems 1 and 2 are upper bounds. The connected equality characterization in Theorem 1 and the tree corollary following it also require correction, as does the minimum in the corollary following Theorem 2.

We also correct the formulas in [2] for the Wiener and Harary indices of their meteor trees. These corrections do not affect their disproof of the conjecture that the path maximizes $W(T)H(T)$.

All graphs in this note are finite, simple, and undirected. For a vertex v, let d_v denote its degree.

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1 The printed inequality and its correction

Let p be a positive integer, let $x_1, \dots, x_p$ be positive real numbers, and define

$$a = \min_{1 \le i \le p} x_i, \qquad A = \max_{1 \le i \le p} x_i.$$

Lemma 1 of [1] states

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

The direction in (1) is reversed. For $(x_1, x_2, x_3) = (1, 1, 2)$, its left side is 10, whereas its right side is $81/8$. The factor involving a and A is an upper bound, not a lower bound.

Lemma 1. *Let $x_1, \dots, x_p$ be positive real numbers, and let*

$$a = \min_{1 \le i \le p} x_i, \qquad A = \max_{1 \le i \le p} x_i.$$

Then

$$p^2 \le \left(\sum_{i=1}^{p} x_i \right) \left(\sum_{i=1}^{p} \frac{1}{x_i} \right) \le \frac{(A+a)^2}{4aA} \, p^2.$$

Equality in the lower bound holds if and only if $x_1 = \cdots = x_p$. Equality in the upper bound is automatic when $a = A$. If $a < A$, equality in the upper bound holds if and only if p is even and exactly $p/2$ of the numbers x_i are equal to a, while the other $p/2$ are equal to A.

Proof. The lower bound is the Cauchy–Schwarz inequality

$$\left(\sum_{i=1}^{p} x_i \right) \left(\sum_{i=1}^{p} \frac{1}{x_i} \right) \ge \left(\sum_{i=1}^{p} 1 \right)^2 = p^2.$$

Equality holds if and only if the vectors $(\sqrt{x_i})_{i=1}^{p}$ and $(1/\sqrt{x_i})_{i=1}^{p}$ are proportional, which is equivalent to $x_1 = \cdots = x_p$.

For every i,

$$(x_i - a)(A - x_i) \ge 0.$$

After division by $x_i > 0$, this becomes

$$x_i + \frac{aA}{x_i} \le a + A.$$

Writing

$$S = \sum_{i=1}^{p} x_i, \qquad T = \sum_{i=1}^{p} \frac{1}{x_i},$$

and summing the preceding inequalities gives

$$S + aAT \le p(a + A).$$

On the other hand, the arithmetic–geometric mean inequality gives

$$S + aAT \ge 2\sqrt{aAST}.$$

Consequently

$$ST \le \frac{(A + a)^2}{4aA}\, p^2.$$

Equality in this upper bound requires equality in both preceding inequalities. Equality in $S + aAT \le p(a + A)$ holds exactly when each x_i belongs to $\{a, A\}$, and equality in the arithmetic–geometric mean step holds exactly when $S = aAT$. If $a < A$ and exactly k of the x_i are equal to A, then

$$S = kA + (p - k)a, \qquad aAT = ka + (p - k)A.$$

Thus $S = aAT$ is equivalent to

$$(2k - p)(A - a) = 0,$$

so $k = p/2$. If $k = p/2$, both inequalities used in the upper-bound proof are equalities. If $a = A$, all x_i are equal and both bounds are equalities. ■

2 Correction to Theorem 1 and its corollary

Let

$$TI(G) = \sum_{uv \in E(G)} F(d_u, d_v), \qquad RTI(G) = \sum_{uv \in E(G)} \frac{1}{F(d_u, d_v)},$$

where F is symmetric and positive on the degree pairs that occur, and suppose $m = |E(G)| \geq 1$. Set

$$F_{\max} = \max_{uv \in E(G)} F(d_u, d_v), \qquad F_{\min} = \min_{uv \in E(G)} F(d_u, d_v).$$

Applying Lemma 1 to the m edge terms gives

$$m^2 \leq TI(G)RTI(G) \leq \frac{(F_{\max} + F_{\min})^2}{4F_{\min}F_{\max}}\, m^2.$$

Theorem 1 of [1] prints only the reverse inequality

$$TI(G)RTI(G) \geq \frac{(F_{\max} + F_{\min})^2}{4F_{\min}F_{\max}}\, m^2.$$

Thus its displayed lower bound is the corrected upper bound, while the correct universal lower bound is m^2. Equality in the lower bound holds if and only if $F(d_u, d_v)$ is constant on $E(G)$. Equality in the upper bound is automatic if $F_{\min} = F_{\max}$. If $F_{\min} < F_{\max}$, equality in the upper bound holds if and only if m is even, exactly $m/2$ edges have edge term $F_{\min}$, exactly $m/2$ edges have edge term $F_{\max}$, and no edge has an intermediate edge term.

For arbitrary positive F, equality need not impose any graph structure. If F is constant, every graph with at least one edge attains equality.

For the first Zagreb and harmonic indices, put $F(d_u, d_v) = d_u + d_v$. Since

$$Zg_1(G) = \sum_{uv \in E(G)} F(d_u, d_v), \qquad Harm(G) = 2 \sum_{uv \in E(G)} \frac{1}{F(d_u, d_v)},$$

the correct estimate is

$$2m^2 \leq Zg_1(G)Harm(G) \leq 2\frac{(F_{\max}+F_{\min})^2}{4F_{\min}F_{\max}}\,m^2,$$

with the same equality conditions for the underlying edge terms.

The connected equality cases

Theorem 1 of [1] states that a connected graph attains the lower bound if and only if it is regular or complete bipartite. This fails because equality only requires $F(d_u, d_v)$ to be constant on $E(G)$, which does not force the graph to be complete bipartite.

For the Sombor index and its reciprocal, write

$$SO(G) = \sum_{uv\in E(G)} \sqrt{d_u^2+d_v^2}, \qquad {}^{m}SO(G) = \sum_{uv\in E(G)} \frac{1}{\sqrt{d_u^2+d_v^2}}.$$

The Sombor pair gives a counterexample. Let G be the bipartite graph with vertex set

$$\{0,1,2,3,4,5\}\cup\{6,7,8,9\}$$

and edge set

$$\begin{aligned} E(G) = \{&\{0,6\},\{0,7\},\{1,7\},\{1,8\},\{2,8\},\{2,9\},\{3,9\},\{3,6\},\\ &\{4,6\},\{4,8\},\{5,7\},\{5,9\}\}. \end{aligned}$$

The vertices $0,1,2,3,6,7,8,9$ lie on the cycle

$$6-0-7-1-8-2-9-3-6,$$

and vertices 4 and 5 are each adjacent to vertices of this cycle, so G is connected. Its degrees are

$$d_0 = d_1 = d_2 = d_3 = d_4 = d_5 = 2, \qquad d_6 = d_7 = d_8 = d_9 = 3.$$

Thus every edge has degree pair $(2, 3)$. Since $m = 12$,

$$SO(G) = 12\sqrt{13}, \qquad {}^{m}SO(G) = \frac{12}{\sqrt{13}},$$

and hence

$$SO(G)\,{}^{m}SO(G) = 144 = m^2.$$

The graph is neither regular nor complete bipartite: its two bipartition classes have sizes 6 and 4, whereas it has 12 edges rather than $6 \cdot 4 = 24$ edges.

A connected bipartite graph is called semiregular if all vertices in each bipartition class have a common degree, with the two common degrees not necessarily equal.

Proposition 1. *Let $F : (\mathbb{Z}_{>0})^2 \longrightarrow \mathbb{R}_{>0}$ be symmetric, and suppose that $x \mapsto F(x, y)$ is injective for every positive integer y. If G is a connected graph with at least one edge, then equality in*

$$TI(G)RTI(G) \geq |E(G)|^2$$

holds if and only if G is regular or semiregular bipartite.

Proof. By Lemma 1, equality holds if and only if $F(d_u, d_v)$ is constant on the edges. Suppose this condition holds. If $u - v - w$ is a path of length two, symmetry gives

$$F(d_u, d_v) = F(d_v, d_w) = F(d_w, d_v).$$

Injectivity in the first coordinate gives $d_u = d_w$.

Fix a vertex r. Along every path starting at r, the degrees therefore alternate between two values. In particular, all vertices at even distance from r have one common degree, say a, and all vertices at odd distance from r have one common degree, say b.

If G is bipartite, connectedness implies that the even- and odd-distance classes from r are its two bipartition classes. Hence G is semiregular bipartite.

Suppose instead that G is not bipartite, and let $v_0v_1\cdots v_{2k}v_0$ be an odd cycle. The length-two path condition gives $d_{v_i} = d_{v_{i+2}}$, with indices taken modulo $2k+1$. Since 2 is relatively prime to $2k+1$, all vertices on the cycle have the same degree, say q. Let xy be an edge with $d_x = q$. Constancy of the edge terms and symmetry give

$$F(d_y, q) = F(q, d_y) = F(q, q).$$

Injectivity in the first coordinate gives $d_y = q$. Since G is connected, induction along paths starting on the cycle shows that every vertex has degree q. Hence G is regular.

Conversely, every regular graph and every semiregular bipartite graph has the same unordered degree pair on every edge. Hence its edge term is constant and equality holds. ■

The injectivity hypothesis of Proposition 1 applies to five of the six pairs listed in [1]. Up to taking a reciprocal or multiplying by a positive constant, the relevant edge functions are

$$x+y, \qquad \sqrt{x+y}, \qquad \sqrt{xy}, \qquad \frac{xy}{x+y}, \qquad \sqrt{x^2+y^2}.$$

Each is strictly increasing in x for fixed $y > 0$. Consequently, if G is connected and has at least one edge, then for the sum-connectivity–Nirmala, Randić–reciprocal Randić, inverse sum indeg–redefined first Zagreb, and Sombor–modified Sombor pairs, equality in the lower bound $TI(G)RTI(G) \geq m^2$ holds if and only if G is regular or semiregular bipartite. For the Zagreb–harmonic pair, the same graphs are exactly the equality cases in

$$Zg_1(G)Harm(G) \geq 2m^2,$$

because $Harm(G)/2$ is the termwise reciprocal of $Zg_1(G)$.

The geometric–arithmetic pair has a different equality classification. Its two indices are

$$GA(G) = \sum_{uv\in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}, \qquad AG(G) = \sum_{uv\in E(G)} \frac{d_u + d_v}{2\sqrt{d_u d_v}}.$$

Proposition 2. *Let G be a connected graph with at least one edge. Then*

$$GA(G)AG(G) = |E(G)|^2$$

if and only if either G is regular, or there exist a rational number $q > 1$, an integer $k \geq 1$, and a positive integer δ such that the degrees occurring in G are exactly

$$\delta, \delta q, \ldots, \delta q^k,$$

all these numbers are integers, and every edge joins vertices whose degrees are consecutive terms of this sequence.

Proof. For $r \geq 1$, set

$$\phi(r) = \frac{2\sqrt{r}}{1+r}.$$

If x, y are positive, then

$$\frac{2\sqrt{xy}}{x+y} = \phi\left(\frac{\max\{x,y\}}{\min\{x,y\}}\right).$$

Differentiation gives

$$\phi'(r) = \frac{1-r}{\sqrt{r}(1+r)^2},$$

so ϕ is strictly decreasing on $[1, \infty)$.

Equality in the Cauchy–Schwarz lower bound holds if and only if the geometric–arithmetic edge term is constant. It follows from the strict monotonicity of ϕ that there is a fixed $q \geq 1$ such that

$$\frac{\max\{d_u, d_v\}}{\min\{d_u, d_v\}} = q \tag{2}$$

for every edge uv. If $q = 1$, adjacent vertices have the same degree, and connectedness implies that G is regular.

Suppose that $q > 1$. Fix a vertex v_0. Along any path beginning at v_0, (2) shows that the degrees have the form $d_{v_0} q^j$, where the integer exponent changes by 1 or -1 at each edge. Since $q > 1$, an exponent is uniquely determined by the resulting degree. Hence every vertex has a well-defined integer exponent, independent of the path chosen from v_0.

Let s and t be the minimum and maximum exponents that occur, put $k = t - s$, and set $\delta = d_{v_0} q^s$. Both δ and every δq^i that occurs are vertex degrees and hence positive integers. A path from a vertex of exponent s to one of exponent t changes its exponent by 1 or -1 at each step, so it visits every exponent between s and t. Therefore the degrees occurring in G are exactly

$$\delta, \delta q, \ldots, \delta q^k.$$

Every edge joins consecutive levels by (2), and q is rational because it is the ratio of the two integer endpoint degrees of any edge. Since G is not regular, $k \geq 1$.

Conversely, suppose that the stated degree-layer structure holds. The ratio of the endpoint degrees of every edge is q, so every geometric–arithmetic edge term equals $\phi(q)$. All edge terms are thus constant, and equality follows from Cauchy–Schwarz. ■

The even and odd degree levels give a bipartition. When $k = 1$, the graph is semiregular bipartite; when $k > 1$, it has more than two degree levels and is not semiregular.

Corollary. *Let $S_n = K_{1,n-1}$ denote the star on n vertices, and let T be a tree on $n \geq 2$ vertices. Then*

$$SO(T)\, {}^m SO(T) \geq (n-1)^2,$$

with equality if and only if $T \cong S_n$.

Proof. The lower bound follows from Proposition 1 because $|E(T)| = n-1$. Suppose equality holds. By that proposition, T is regular or semiregular bipartite. Every finite tree on at least two vertices has a leaf. If T is regular, it is therefore 1-regular and hence $T \cong K_2 = S_2$. If T is semiregular bipartite, the bipartition class containing a leaf has common degree 1. If the other bipartition class contained two vertices, the unique path between them would contain an internal vertex in the degree-1 class, a contradiction. Thus the other class has one vertex and T is a star. Conversely, every star is semiregular bipartite, so equality holds. ■

For each of the other three exact reciprocal pairs covered by Proposition 1, the leaf argument in the preceding corollary shows that the product on n-vertex trees has minimum $(n-1)^2$, attained exactly by S_n. For the Zagreb–harmonic pair, the minimum is $2(n-1)^2$, again attained exactly by S_n.

Correction to the tree corollary

Let $n \geq 2$, and fix a positive symmetric function F of the endpoint degrees. The corollary following Theorem 1 of [1] asserts that the minimum of $TI(T)RTI(T)$ over n-vertex trees is $(n-1)^2$, attained if and only if $T \cong S_n$, where $S_n = K_{1,n-1}$. The minimum value and the sufficiency of the star are correct. Lemma 1 gives

$$TI(T)RTI(T) \geq |E(T)|^2 = (n-1)^2,$$

and S_n attains equality because all its edges have the same degree pair. This uniqueness assertion does not hold for every F. Equality only requires $F(d_u, d_v)$ to be constant on $E(T)$.

Let T be obtained from $K_{1,4}$ by subdividing each edge once. Then T has nine vertices and eight edges. Four edges have degree pair $(4, 2)$, and four have degree pair $(2, 1)$. For the geometric–arithmetic edge term,

$$\frac{2\sqrt{d_u d_v}}{d_u + d_v},$$

both degree pairs give the same value:

$$\frac{2\sqrt{4 \cdot 2}}{4+2} = \frac{2\sqrt{2 \cdot 1}}{2+1} = \frac{2\sqrt{2}}{3}.$$

The reciprocal arithmetic–geometric term is therefore $3/(2\sqrt{2})$ on every edge. Consequently,

$$GA(T) = 8 \cdot \frac{2\sqrt{2}}{3} = \frac{16\sqrt{2}}{3}, \qquad AG(T) = 8 \cdot \frac{3}{2\sqrt{2}} = 6\sqrt{2},$$

and hence

$$GA(T)AG(T) = 64 = |E(T)|^2 = (9-1)^2.$$

The tree T attains the minimum but is not a star. Thus the uniqueness assertion in the published corollary fails for the geometric–arithmetic pair.

3 Correction to Theorem 2 and its corollary

Let G be a connected graph on $n \geq 2$ vertices, let

$$N = \binom{n}{2},$$

and let D be the diameter of G. For vertices u and v, let $d(u,v)$ denote their graph distance. We use the convention

$$W(G) = \sum_{\{u,v\} \in \binom{V(G)}{2}} d(u,v), \qquad H(G) = \sum_{\{u,v\} \in \binom{V(G)}{2}} \frac{1}{d(u,v)}.$$

Theorem 2 of [1] states

$$W(G)H(G) \geq \frac{(D+1)^2}{4D} \binom{n}{2}^2. \tag{3}$$

The direction in (3) is reversed. Applying Lemma 1 to the N unordered pairwise distances gives the corrected two-sided estimate

$$N^2 \leq W(G)H(G) \leq \frac{(D+1)^2}{4D}\, N^2.$$

Equality in the lower bound holds if and only if all pairwise distances are equal. Because a connected graph has an adjacent pair, the common distance must then be 1, so equality holds if and only if $G \cong K_n$. Consequently, the minimum of $W(G)H(G)$ over connected n-vertex graphs is

$$\left(\binom{n}{2}\right)^2,$$

not $n(n-1)/2$ as stated in the corollary following Theorem 2 of [1]. The complete graph attains the corrected value because $W(K_n) = H(K_n) = \binom{n}{2}$.

For the upper bound, if $D = 1$, then $G \cong K_n$ and equality is automatic. Suppose $D > 1$. The equality condition in Lemma 1 requires every pairwise distance to be either 1 or D, with exactly $N/2$ pairs of each type. This is impossible when $D \geq 3$, because a diametral path contains two vertices at distance 2. Hence, for $D > 1$, equality in the upper bound holds if and only if

$$D = 2 \qquad \text{and} \qquad |E(G)| = \frac{1}{2}\binom{n}{2}.$$

The noncomplete graph C_5, for example, attains this bound, so K_n is not the only equality case.

The displayed bound in the original Theorem 2 fails for the three-vertex path P_3: its pairwise distances are $1, 1, 2$, and therefore

$$W(P_3)H(P_3) = 4 \cdot \frac{5}{2} = 10 < \frac{(2+1)^2}{4 \cdot 2}\binom{3}{2}^2 = \frac{81}{8}.$$

4 The maximum over trees

Li, Li, and Liu [2] disproved the conjecture in [1] that the path maximizes $W(T)H(T)$, but did not determine the maximum. Their proof uses a family of meteor trees, but the final simplified formulas for both indices of these trees contain algebraic errors. We correct these formulas below and determine the leading asymptotic term of the maximum. Let

$$M_n = \max\{W(T)H(T) : T \text{ is a tree of order } n\}.$$

Theorem 3. *We have*

$$\lim_{n\to\infty} \frac{M_n}{n^5} = \frac{102 + 7\sqrt{21}}{25000}.$$

Proof. For the lower bound, let $0 \leq k \leq n-2$, and let $B(n,k)$ be obtained from $v_0v_1 \cdots v_L$ by adjoining k leaves to v_0, where $L = n - k - 1$. Write

$h_r = \sum_{j=1}^{r} 1/j$. Partitioning the vertex pairs into two path vertices, a new leaf and a path vertex, and two new leaves gives

$$W(B(n,k)) = \frac{L(L+1)(L+2)}{6} + \frac{k(L+1)(L+2)}{2} + k(k-1)$$

and

$$H(B(n,k)) = (L+1)h_L - L + kh_{L+1} + \frac{k(k-1)}{4}.$$

Fix $0 < \alpha < 1$ and take $k = \lfloor \alpha n \rfloor$. Since $L/n \to 1-\alpha$ and $h_L = O(\log n)$, these identities give

$$\frac{W(B(n,k))H(B(n,k))}{n^5} \longrightarrow f(\alpha) := \frac{\alpha^2(1-\alpha)^2(1+2\alpha)}{24}.$$

For $0 < \alpha < 1$,

$$\frac{f'(\alpha)}{f(\alpha)} = \frac{2}{\alpha} - \frac{2}{1-\alpha} + \frac{2}{1+2\alpha}.$$

This expression has a unique zero, at

$$\alpha_0 = \frac{1+\sqrt{21}}{10},$$

and changes sign from positive to negative there. Direct substitution gives

$$f(\alpha_0) = \frac{102+7\sqrt{21}}{25000}.$$

Since $M_n \geq W(B(n, \lfloor \alpha_0 n \rfloor))H(B(n, \lfloor \alpha_0 n \rfloor))$, the lower bound follows.

We prove the upper bound by partitioning each tree into subtrees of sublinear diameter. Let T be an n-vertex tree, and set

$$r = \lfloor n^{1/4} \rfloor, \qquad \ell = \lfloor n^{1/2} \rfloor.$$

We may assume that n is large enough that $1 \leq r < \ell$. Root T at an arbitrary vertex. For a residue $t \in \{0, 1, \ldots, \ell - 1\}$, delete every edge whose endpoint farther from the root has depth congruent to t modulo ℓ. Let $\mathcal{P}_t$ be the set of components that remain.

Every component in $\mathcal{P}_t$ is connected and has diameter at most 2ℓ. In-

deed, a connected subtree of a rooted tree has a unique vertex of minimum depth. The path from this vertex to any other vertex in the component has fewer than ℓ edges. Otherwise that path would contain an edge whose lower endpoint has depth congruent to t modulo ℓ. Hence every vertex is at distance less than ℓ from the minimum-depth vertex, so the triangle inequality gives diameter less than 2ℓ.

Let $\mathcal{C}_r$ be the set of unordered vertex pairs at distance at most r. Choose t uniformly from $\{0, 1, \ldots, \ell - 1\}$. If $\{u, v\} \in \mathcal{C}_r$, then u and v lie in different components only if an edge of their path is deleted. Each edge is deleted for exactly one value of t, so the union bound gives

$$\Pr\big(u \text{ and } v \text{ lie in different components}\big) \le \frac{d_T(u,v)}{\ell} \le \frac{r}{\ell}.$$

This remains an upper bound if several path edges have the same residue, since repeated residues only reduce the number of values of t that separate the pair. Consequently, some residue t separates at most

$$\frac{r}{\ell}|\mathcal{C}_r| \le \frac{r}{\ell}\binom{n}{2} \tag{4}$$

pairs in $\mathcal{C}_r$. Fix such a residue, and let the component orders of $\mathcal{P}_t$ be $c_1, c_2, \ldots$.

We first bound the Harary index. The $n - 1$ adjacent pairs contribute $n - 1$. A nonadjacent pair at distance at most r contributes at most $1/2$, and a pair at distance greater than r contributes at most $1/r$. Every pair in $\mathcal{C}_r$ either lies in one component or is among the pairs counted in (4). Therefore

$$H(T) \le n - 1 + \frac{1}{2}\sum_j \binom{c_j}{2} + \frac{r}{2\ell}\binom{n}{2} + \frac{1}{r}\binom{n}{2}.$$

This estimate deliberately overcounts: adjacent pairs may also occur in the component or separation terms, and the last binomial coefficient includes pairs at distance at most r. Both overcounts preserve the upper bound.

Since $\binom{c_j}{2} \le c_j^2/2$, division by n^2 yields

$$\frac{H(T)}{n^2} \le \frac{1}{4}\sum_j \left(\frac{c_j}{n}\right)^2 + \frac{r}{4\ell} + \frac{1}{2r} + \frac{1}{n}. \tag{5}$$

Fix $0 < \varepsilon < 1$. Relabel the components so that the heavy components, those of order at least εn, have orders c_i for $1 \le i \le k$, and put

$$A = \sum_{i=1}^{k} \frac{c_i}{n}, \qquad s = 1 - A, \qquad Q = \sum_{i=1}^{k} \left(\frac{c_i}{n}\right)^2. \tag{6}$$

There are at most $1/\varepsilon$ heavy components. For the remaining components,

$$\sum_{j>k} \left(\frac{c_j}{n}\right)^2 < \varepsilon \sum_{j>k} \frac{c_j}{n} \le \varepsilon.$$

Define

$$\eta_n = \frac{r}{4\ell} + \frac{1}{2r} + \frac{1}{n}.$$

Then $\eta_n \to 0$. It follows from (5) that

$$\frac{H(T)}{n^2} \le \frac{Q + \varepsilon}{4} + \eta_n, \tag{7}$$

where η_n is independent of T and ε.

We next bound the Wiener index. Contract each heavy component to a connector vertex c_i^*, and let R be the resulting tree. Let $\pi : V(T) \to V(R)$ be the quotient map, and define

$$\widetilde{W} = \sum_{\{u,v\} \in \binom{V(T)}{2}} d_R(\pi(u), \pi(v)).$$

Contracting pairwise disjoint connected subtrees of a tree yields a tree, so R is a tree. If $k = 0$, all sums over heavy components are empty, $A = Q = 0$, $s = 1$, and no contraction is performed, so $R = T$. A path in T meets each heavy component in a connected segment. Since each heavy

component has diameter at most 2ℓ, for all $u, v \in V(T)$,

$$0 \le d_T(u,v) - d_R(\pi(u),\pi(v)) \le 2k\ell.$$

Thus

$$0 \le W(T) - \widetilde{W} \le 2k\ell\binom{n}{2} \le \frac{\ell n^2}{\varepsilon} = o(n^3), \tag{8}$$

for fixed ε.

Let O be the set of vertices outside the heavy components, and put $N = |O|$. By the definition of A in (6),

$$N = n - \sum_{i=1}^{k} c_i = n(1-A) = sn$$

exactly. The tree R has

$$m = N + k = sn + k$$

vertices. If v is a vertex of an m-vertex tree, then for $1 \le j \le m-1$ at most $m-j$ vertices have distance at least j from v: a geodesic to any such vertex contains j vertices at distance less than j. Summing the distance tails gives

$$\sum_u d(u,v) = \sum_{j=1}^{m-1} |\{u : d(u,v) \ge j\}| \le \sum_{j=1}^{m-1} (m-j) = \frac{m(m-1)}{2}. \tag{9}$$

Induction on m now shows that every m-vertex tree U satisfies

$$W(U) \le \frac{m^3 - m}{6}.$$

The one-vertex case is immediate. For the induction step, delete a leaf from an m-vertex tree. By (9), the sum of its distances to the remaining vertices is at most $m(m-1)/2$, while

$$\frac{m^3-m}{6} - \frac{(m-1)^3-(m-1)}{6} = \frac{m(m-1)}{2}.$$

The contribution to $\widetilde{W}$ from pairs in O is a subsum of $W(R)$, since every vertex of O remains a distinct vertex of R. It is therefore at most $(m^3 - m)/6$. For each i, the pairs with one vertex in the ith heavy component and one vertex in O contribute at most

$$c_i \sum_{v \in O} d_R(c_i^*, v) \le c_i \frac{m(m-1)}{2}.$$

Finally, $d_R(c_i^*, c_j^*) \le m - 1$, so the contribution from pairs in two distinct heavy components is at most

$$(m-1) \sum_{1 \le i < j \le k} c_i c_j = \frac{(m-1)n^2}{2}(A^2 - Q).$$

Pairs within one heavy component contribute zero to $\widetilde{W}$. Combining these estimates gives

$$\widetilde{W} \le \frac{m^3 - m}{6} + \frac{Anm(m-1)}{2} + \frac{(m-1)n^2}{2}(A^2 - Q). \tag{10}$$

For fixed ε, we have $k \le 1/\varepsilon$, so $m = sn + O_\varepsilon(1)$. Equations (8) and (10) therefore give, uniformly over all n-vertex trees,

$$\frac{W(T)}{n^3} \le \frac{s^3}{6} + \frac{As^2}{2} + \frac{s(A^2 - Q)}{2} + \theta_{n,\varepsilon}, \tag{11}$$

where $\theta_{n,\varepsilon} \ge 0$ is independent of T. The contraction error in (8), divided by n^3, is at most $\ell/(\varepsilon n)$, and every error obtained from replacing $m/n = s + k/n$ by s is bounded by C_ε/n for a constant C_ε independent of T. Increasing C_ε if necessary, we may therefore take

$$0 \le \theta_{n,\varepsilon} \le C_\varepsilon \left(\frac{\ell}{n} + \frac{1}{n} \right),$$

so $\theta_{n,\varepsilon} \to 0$ as $n \to \infty$ for each fixed ε.

Since $A = 1 - s$, define

$$\Phi(s, Q) = \frac{s^3}{6} + \frac{(1-s)s^2}{2} + \frac{s((1-s)^2 - Q)}{2}.$$

The parameters in (6) satisfy

$$0 \le s \le 1, \qquad 0 \le Q \le (1-s)^2. \tag{12}$$

Indeed, $Q \ge 0$, and

$$Q = \sum_{i=1}^{k} \left(\frac{c_i}{n}\right)^2 \le \left(\sum_{i=1}^{k} \frac{c_i}{n}\right)^2 = A^2 = (1-s)^2.$$

Multiplying (7) and (11) gives

$$\begin{aligned} \frac{W(T)H(T)}{n^5} \le \frac{Q+\varepsilon}{4}\Phi(s,Q) + \frac{Q+\varepsilon}{4}\theta_{n,\varepsilon} \\ + \Phi(s,Q)\eta_n + \eta_n\theta_{n,\varepsilon}. \end{aligned} \tag{13}$$

On the domain (12), $Q \le 1$ and $0 \le \Phi(s,Q) \le 7/6$. Since $0 < \varepsilon < 1$, the last three terms on the right side of (13) tend to zero uniformly over all T as $n \to \infty$ with ε fixed.

It remains to optimize the term not containing ε. Set

$$C = \frac{s(s^2-3s+3)}{6}.$$

Then

$$\frac{Q}{4}\Phi(s,Q) = \frac{Q}{4}\left(C - \frac{sQ}{2}\right). \tag{14}$$

If $s = 0$ or $s = 1$, this expression is zero. Suppose $0 < s < 1$. If $C \ge s(1-s)^2$, expression (14) is maximized over the interval in (12) at $Q = (1-s)^2$, and its value is

$$\frac{(1-s)^2 s^2(3-2s)}{24} = f(1-s). \tag{15}$$

If $C < s(1-s)^2$, expression (14) is maximized at $Q = C/s$, and its value is

$$g(s) = \frac{s(s^2-3s+3)^2}{288}. \tag{16}$$

Since

$$C - s(1-s)^2 = -\frac{s(5s^2-9s+3)}{6},$$

the second case is $0 < s < s_0$, where

$$s_0 = \frac{9 - \sqrt{21}}{10}.$$

On this interval,

$$g'(s) = \frac{(s^2 - 3s + 3)(5s^2 - 9s + 3)}{288} > 0.$$

Hence $g(s) \le g(s_0)$. In the first case, (15) is at most the maximum of f, which is $f(1 - s_0)$. Direct substitution gives

$$g(s_0) = f(1 - s_0) = \frac{102 + 7\sqrt{21}}{25000}.$$

Therefore

$$\frac{Q}{4}\Phi(s, Q) \le \frac{102 + 7\sqrt{21}}{25000}$$

throughout (12). Also, $\varepsilon\Phi(s, Q)/4 \le 7\varepsilon/24$. Taking the supremum over all n-vertex trees in (13), then letting $n \to \infty$ with ε fixed, gives

$$\limsup_{n\to\infty} \frac{M_n}{n^5} \le \frac{102 + 7\sqrt{21}}{25000} + \frac{7\varepsilon}{24}.$$

Letting $\varepsilon \downarrow 0$ proves the upper bound. ■

We finish by correcting the meteor calculation in [2]. For even $n = 2m$, let $\mathcal{M}_n$ denote the meteor tree used there. It is obtained from disjoint copies of P_m and $S_m = K_{1,m-1}$ by adding an edge between an end vertex of the path and the center of the star. Partitioning the vertex pairs into pairs within the path, pairs within the star, and pairs with one vertex in each gives

$$\begin{aligned} W(\mathcal{M}_n) &= \frac{m^3 - m}{6} + (m-1)^2 + \sum_{j=1}^{m} \big(j + (m-1)(j+1)\big) \\ &= \frac{n^3}{12} + \frac{5n^2}{8} - \frac{19n}{12} + 1. \end{aligned}$$

Writing $h_r = \sum_{j=1}^{r} 1/j$, the same partition gives

$$\begin{aligned} H(\mathcal{M}_n) &= mh_m - m + \frac{m^2+m-2}{4} + h_m + (m-1)(h_{m+1}-1) \\ &= nh_{n/2} + \frac{n^2}{16} - \frac{7n}{8} + \frac{3}{2} - \frac{4}{n+2}. \end{aligned}$$

The unsimplified distance sums in [2] are correct, but their final simplifications are not. They print

$$W(\mathcal{M}_n) = \frac{5n^3}{48} + \frac{5n^2}{8} - \frac{5n}{3} + 1$$

and print the harmonic term in $H(\mathcal{M}_n)$ as $(n/2)h_{n/2}$. The correct coefficients are those displayed above. Consequently,

$$W(\mathcal{M}_n)H(\mathcal{M}_n) = \frac{n^5}{192} + O(n^4 \log n),$$

not $5n^5/768 + O(n^4 \log n)$ as stated there. This correction does not affect the conclusion that, for all sufficiently large even n, the path fails to maximize the product, because $W(P_n)H(P_n) = O(n^4 \log n)$.

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References

[1] I. Gutman, B. Furtula, I. Redžepović, On topological indices and their reciprocals, *MATCH Commun. Math. Comput. Chem.* **91** (2024) 287–297. **doi:** 10.46793/match.91-2.287G

[2] L. Li, X. Li, W. Liu, Note on the product of Wiener and Harary indices, *MATCH Commun. Math. Comput. Chem.* **91** (2024) 299–305 **doi:** 10.46793/match.91-2.299L