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On the Triplet Sombor Index: Corrections and Extremal Results

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Abstract

For a graph G let $\mathcal{T}(G)$ be the set of 3-subsets of $V(G)$ inducing a connected subgraph. The Triplet Sombor index is $\mathrm{TSO}(G) = \sum_{\{u,v,w\}\in\mathcal{T}(G)} \sqrt{d_u^2 + d_v^2 + d_w^2}$. We correct several inaccuracies in the existing literature on this index and obtain exact formulas for the number of connected triples and for two weighted sums over them. Among connected graphs of order n, we show that the path is the unique minimizer of TSO and the complete graph the unique maximizer. For an r-regular graph G with $t(G)$ triangles, we prove $\mathrm{TSO}(G) = \frac{\sqrt{3}}{2} nr^2(r-1) - 2\sqrt{3}\, r\, t(G)$. We also show that TSO is monotone under edge addition and under passing to subgraphs, which yields lower bounds in terms of the maximum degree, longest path, circumference and clique number.

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1 Introduction

All graphs are finite and simple. For $G = (V, E)$ write $n = |V|$, $m = |E|$, let δ and Δ be the minimum and maximum degree, and let $t(G)$ be the number of triangles. Gutman [2] introduced the Sombor index $\mathrm{SO}(G) = \sum_{uv \in E} \sqrt{d_u^2 + d_v^2}$. For the related degree-ratio Sombor index, see [1, 3]. Sultan, Shaveisi and Edalatzadeh [4] replaced edges by connected triples and defined

$$\mathrm{TSO}(G) = \sum_{\{u,v,w\} \in \mathcal{T}(G)} \sqrt{d_u^2 + d_v^2 + d_w^2}.$$

A 3-set is connected exactly when it spans a path $a - v - b$ or a triangle, so TSO is controlled by the wedges (pairs of neighbours of a vertex) and the triangles of G. We use this throughout.

In Section 2 we prove exact identities for the number of connected triples and for two weighted sums over them, and derive basic bounds. Section 3 corrects the statements of [4] that are inaccurate or insufficiently proved (Example 1 and Tables 1–2, Theorem 2, the proofs of Theorems 3, 5 and 6, and the data of Section 4). Theorems 3, 5 and 6 of [4] are true, and we supply valid proofs. Section 4 contains new results: an exact formula for regular graphs, monotonicity under edge addition and under passing to subgraphs, and the extremal bounds $\mathrm{TSO}(P_n) \le \mathrm{TSO}(G) \le \mathrm{TSO}(K_n)$ for connected G. Section 5 lists open problems.

2 Preliminaries

A *wedge* $(v; a, b)$ is a pair $\{a, b\}$ of distinct neighbours of a vertex v, its centre. The number of wedges is $\omega(G) = \sum_v \binom{d_v}{2} = \big(\sum_v d_v^2 - 2m\big)/2$. For a 3-set $X = \{u, v, w\}$ put $S(X) = d_u + d_v + d_w$, $q(X) = d_u^2 + d_v^2 + d_w^2$ and $\rho(X) = \sqrt{q(X)}$, so that $\mathrm{TSO}(G) = \sum_{X \in \mathcal{T}(G)} \rho(X)$. Let

$$\tau(G) = |\mathcal{T}(G)|, \qquad D_{\mathcal{T}}(G) = \sum_{X \in \mathcal{T}(G)} S(X), \qquad Q_{\mathcal{T}}(G) = \sum_{X \in \mathcal{T}(G)} q(X),$$

$$M_1 = \sum_v d_v^2, \quad M_2 = \sum_{uv\in E} d_u d_v, \quad \Phi_3 = \sum_v d_v^3,$$
$$\Phi_4 = \sum_v d_v^4, \quad Z = \sum_{uv\in E} d_u d_v (d_u + d_v).$$

Lemma 1. *A 3-set X induces a connected subgraph if and only if it spans at least two edges. In that case X is either an induced path $a-v-b$, which corresponds to exactly one wedge, or a triangle, which corresponds to three wedges. Hence $\omega(G) = \tau(G) + 2t(G)$, and for every function f on 3-sets*

$$\sum_{X\in\mathcal{T}(G)} f(X) = \sum_{(v;a,b)} f(\{v,a,b\}) - 2\sum_{\triangle} f(\triangle),$$

the first sum being over all wedges and the second over all triangles.

Proof. A 3-set with at most one edge is disconnected; with two or three edges it is connected. An induced path arises from one wedge and a triangle from three. ■

Lemma 2. *If H is a spanning subgraph of G, then $\mathcal{T}(H) \subseteq \mathcal{T}(G)$. If $X \in \mathcal{T}(G)$, then $\rho(X) \geq \sqrt{6}$.*

Proof. Adding edges cannot disconnect an induced subgraph. In a connected 3-set some vertex is adjacent to the other two, so its degree is at least 2 and the others have degree at least 1; thus $q(X) \geq 4+1+1$. ■

For a function g on V,

$$\sum_{(v;a,b)} \big(g(v)+g(a)+g(b)\big) = \sum_v \binom{d_v}{2} g(v) + \sum_{uv\in E} \big[(d_u-1)g(v)+(d_v-1)g(u)\big], \tag{1}$$

since v is the centre of $\binom{d_v}{2}$ wedges, and a vertex a is an end of $d_v - 1$ wedges centred at each neighbour v of a.

Theorem 1. *For every graph G,*

$$\tau(G) = \frac{M_1 - 2m}{2} - 2t(G),$$
$$D_{\mathcal{T}}(G) = 2M_2 - \tfrac{3}{2}M_1 + \tfrac{1}{2}\Phi_3 - 2\sum_{uvw\in\triangle} (d_u + d_v + d_w),$$

$$Q_{\mathcal{T}}(G) = \tfrac{1}{2}\Phi_4 - \tfrac{3}{2}\Phi_3 + Z - 2\sum_{uvw\in\triangle}(d_u^2 + d_v^2 + d_w^2).$$

If G is triangle-free, in particular if G is a tree, the triangle sums vanish.

Proof. The first identity is Lemma 1. Take $g(v) = d_v$ in (1). The first sum equals $\frac{1}{2}(\Phi_3 - M_1)$ and the second equals $\sum_{uv\in E}(2d_u d_v - d_u - d_v) = 2M_2 - M_1$. Now apply Lemma 1 with $f = S$. For the third identity take $g(v) = d_v^2$: the first sum is $\frac{1}{2}(\Phi_4 - \Phi_3)$, the second is $\sum_{uv\in E}\big[(d_u - 1)d_v^2 + (d_v - 1)d_u^2\big] = Z - \Phi_3$, and we apply Lemma 1 with $f = q$. ∎

If T is a tree, every connected triple is a wedge, and

$$\mathrm{TSO}(T) = \sum_v \sum_{\{a,b\}\subseteq N(v)} \sqrt{d_v^2 + d_a^2 + d_b^2}. \tag{2}$$

Theorem 2. *Let $\mathcal{T}(G) \neq \emptyset$. Then*

(i) $\mathrm{TSO}(G) \geq D_{\mathcal{T}}/\sqrt{3}$;

(ii) $\mathrm{TSO}(G) \leq \sqrt{\tau\, Q_{\mathcal{T}}} \leq \sqrt{\Delta\,\tau\, D_{\mathcal{T}}}$;

(iii) $\mathrm{TSO}(G) \geq Q_{\mathcal{T}}/(\sqrt{3}\,\Delta)$.

Equality in (i) holds if and only if the three degrees agree in every connected triple; if G is connected of order at least 3, this means that G is regular. Equality in the first inequality of (ii) holds if and only if q is constant on $\mathcal{T}(G)$. If G is connected, equality in the second inequality of (ii) and in (iii) holds if and only if G is regular.

Proof. (i) By the quadratic–arithmetic mean inequality, $\rho(X) \geq S(X)/\sqrt{3}$ with equality if and only if the three degrees agree. Summing over $\mathcal{T}(G)$ gives (i). Suppose G is connected, $n \geq 3$, and the degrees agree in each connected triple. For an edge uv there is a vertex z adjacent to u or v, and $\{u, v, z\}$ is connected, so $d_u = d_v$. Hence G is regular. The converse is clear.

(ii) By Cauchy–Schwarz, $\sum_X \rho(X) \leq \sqrt{\tau \sum_X \rho(X)^2}$, with equality if and only if ρ is constant on $\mathcal{T}(G)$. Moreover $d_x^2 \leq \Delta d_x$ gives $q(X) \leq \Delta S(X)$, so $Q_{\mathcal{T}} \leq \Delta D_{\mathcal{T}}$. Equality forces $d_x = \Delta$ for each vertex x lying in a connected triple, and in a connected graph of order ≥ 3 every vertex does.

(iii) Since $\rho(X) \le \sqrt{3}\Delta$, we have $q(X) \le \sqrt{3}\Delta\,\rho(X)$; sum over $\mathcal{T}(G)$. Equality needs $\rho(X) = \sqrt{3}\Delta$ for all X. ∎

Remark. The first inequality in (ii) is sharper than $\sqrt{\Delta\tau D_{\mathcal{T}}}$, and it is attained by non-regular graphs. All connected triples of the star $K_{1,n-1}$ have the same weight; so do those of P_4 (where $q = 9$) and of the friendship graph Fr_k, k triangles sharing a vertex (every connected triple contains the centre and has $q = 4k^2 + 8$).

Corollary. *If $\mathcal{T}(G) \neq \emptyset$, then*

$$\frac{1}{\sqrt{3}}\Big(2M_2 - \tfrac{3}{2}M_1 + \tfrac{1}{2}\Phi_3 - 2\sum_{uvw\in\triangle}(d_u + d_v + d_w)\Big) \le \mathrm{TSO}(G) \le \sqrt{\tau(G)\,Q_{\mathcal{T}}(G)},$$

with $\tau(G)$ and $Q_{\mathcal{T}}(G)$ as in Theorem 1. In particular, if G is triangle-free (for instance a tree),

$$\mathrm{TSO}(G) \ge \frac{1}{\sqrt{3}}\Big(2M_2 - \tfrac{3}{2}M_1 + \tfrac{1}{2}\Phi_3\Big).$$

Proof. Combine Theorem 1 with Theorem 2(i) and the first inequality of (ii). ∎

These bounds are expressed through $M_1, M_2, \Phi_3, \Phi_4, Z$, the number of edges and the triangles of G, rather than through n, Δ and δ alone as in [4]. For P_4 we have $M_1 = 10$, $M_2 = 8$, $\Phi_3 = 18$, and the bound reads $10/\sqrt{3} \approx 5.77 \le 6 = \mathrm{TSO}(P_4)$.

3 Corrections to published results

Items (iii) and (v) of Example 1 in [4], and the numerical tables, contain errors.

Remark. (a) For paths, [4] gives $\mathrm{TSO}(P_n) = 6 + 2\sqrt{3}\,(n-4)$ for $n \ge 4$, which is correct, but the tabulated values for $n = 4, 5, 6, 7$ are $6+2\sqrt{3}$, $6+4\sqrt{3}$, $6+4\sqrt{3}$, $6+4\sqrt{3}$, while the formula gives 6, $6+2\sqrt{3}$, $6+4\sqrt{3}$, $6+6\sqrt{3}$. Only the entry for $n = 6$ is right; the entry $\sqrt{6}$ for $n = 3$ is also right.

(b) The formula $\mathrm{TSO}(C_n) = 2\sqrt{3}\,n$ is stated for all $n \geq 3$. Since $C_3 = K_3$ has a single connected triple, $\mathrm{TSO}(C_3) = 2\sqrt{3}$, not $6\sqrt{3}$. (Table 1 of [4] has the correct value, contradicting the formula.)

(c) For complete bipartite graphs [4] gives

$$a\binom{b}{2}\sqrt{a^2+2b^2} + b\binom{a}{2}\sqrt{b^2+2a^2}.$$

The radicals are interchanged: a vertex on the side of size a has degree b, and its two partners have degree a. For $K_{2,3}$ the formula of [4] yields $6\sqrt{22} + 3\sqrt{17} \approx 40.51$, whereas $K_{2,3}$ has six connected triples of weight $\sqrt{17}$ and three of weight $\sqrt{22}$, so $\mathrm{TSO}(K_{2,3}) = 6\sqrt{17} + 3\sqrt{22} \approx 38.81$.

Proposition 3. *(i)* $\mathrm{TSO}(P_3) = \sqrt{6}$ *and* $\mathrm{TSO}(P_n) = 6 + 2\sqrt{3}\,(n-4)$ *for* $n \geq 4$*; for* $n = 3, \ldots, 7$ *the values are* $\sqrt{6},\ 6,\ 6+2\sqrt{3},\ 6+4\sqrt{3},\ 6+6\sqrt{3}$.

(ii) $\mathrm{TSO}(C_n) = 2\sqrt{3}\,n$ *for* $n \geq 4$, *and* $\mathrm{TSO}(C_3) = 2\sqrt{3}$.

(iii) For $a, b \geq 1$, $\mathrm{TSO}(K_{a,b}) = a\binom{b}{2}\sqrt{b^2+2a^2} + b\binom{a}{2}\sqrt{a^2+2b^2}$.

(iv) $\mathrm{TSO}(K_n) = \sqrt{3}\binom{n}{3}(n-1) = \frac{\sqrt{3}}{6}\,n(n-1)^2(n-2)$ *and* $\mathrm{TSO}(K_{1,n-1}) = \binom{n-1}{2}\sqrt{(n-1)^2+2}$.

Proof. (i) The two triples containing an end vertex have degrees $(1,2,2)$ and weight 3; the other $n-4$ triples have weight $\sqrt{12}$. (ii) For $n \geq 4$ the connected triples are the n sets of three consecutive vertices, each of weight $\sqrt{12}$. (iii) A connected triple has two vertices on one side and one on the other, and the single vertex is adjacent to both others. If it lies on the side of size a, there are $a\binom{b}{2}$ such triples, its degree is b, the other two have degree a, and the weight is $\sqrt{b^2+2a^2}$. The other case is symmetric. (iv) is immediate. ∎

Theorem 2 of [4] asserts that for connected G of order n,

$$\mathrm{TSO}(G) \leq \frac{\sqrt{3}}{2}\,n\Delta^2(\Delta-1), \qquad \mathrm{TSO}(G) \geq \begin{cases} \frac{\sqrt{3}}{6}\,n\delta^2(\delta-1), & \delta \geq 2, \\ (n-2)\sqrt{6}, & \delta = 1, \end{cases}$$

and the Remark following it claims that equality holds in the upper bound if and only if G is Δ-regular.

Remark. The upper bound is correct, the equality clause is not. The proof counts $n\binom{\Delta}{2}$ wedges, but a triangle contains three wedges and yields one connected triple. For the 3-regular graph K_4 the bound is $36\sqrt{3} \approx 62.35$, while $\mathrm{TSO}(K_4) = 12\sqrt{3} \approx 20.78$. Equality holds if and only if G is Δ-regular and triangle-free. The last sentence of that Remark, on maximizers when no Δ-regular graph of order n exists, is not a precise statement ("the largest possible number of vertices of degree Δ" does not determine the maximizers) and is not proved. In the proof of the lower bound, the inequality $\tau \geq \frac{n}{3}\binom{\delta}{2}$ is asserted as "clear"; it requires $\omega \leq 3\tau$ (Lemma 1). For $\delta = 1$ the bound $\tau \geq n - 2$ is justified by the claim that the path minimizes the number of connected triples, which [4] establishes only for trees; for general G one passes to a spanning tree and uses Lemma 2. The equality case of the lower bound is not discussed.

Proposition 4. *Let G be a connected graph of order $n \geq 3$. Then*

$$\mathrm{TSO}(G) \leq \sqrt{3}\,\Delta\Big(\frac{n\Delta(\Delta-1)}{2} - 2t(G)\Big) \leq \frac{\sqrt{3}}{2}\,n\Delta^2(\Delta-1).$$

Equality holds in the first inequality if and only if G is Δ-regular, and in the second if and only if, in addition, G is triangle-free. If $\delta \geq 2$, then

$$\mathrm{TSO}(G) \geq \sqrt{3}\,\delta\,\tau(G) \geq \frac{\sqrt{3}}{6}\,n\delta^2(\delta-1),$$

with equality in the last bound if and only if $G = K_n$. For every $\delta \geq 1$ we have $\tau(G) \geq n - 2$ and $\mathrm{TSO}(G) \geq (n-2)\sqrt{6}$.

Proof. Each connected triple has $\rho \leq \sqrt{3}\Delta$, and $\tau = \omega - 2t \leq n\binom{\Delta}{2} - 2t$. If equality holds in the first inequality, every vertex (each lies in a connected triple) has degree Δ. Conversely, in a Δ-regular graph $\rho(X) = \sqrt{3}\Delta$ for all X and $\omega = n\binom{\Delta}{2}$. The second inequality is $t \geq 0$.

For the lower bound, $\rho(X) \geq \sqrt{3}\delta$, and $\omega \leq 3\tau$ with equality if and only if every connected triple is a triangle (Lemma 1). Hence $\tau \geq \omega/3 \geq \frac{n}{3}\binom{\delta}{2}$. Equality in the last bound forces δ-regularity and that every connected triple be a triangle; then no two vertices are at distance two, so $G = K_n$. Finally, a spanning tree T of G satisfies $\mathcal{T}(T) \subseteq \mathcal{T}(G)$ by Lemma 2, and

with $\varepsilon_v = d_v - 1$ we get $\tau(T) = \sum_v \binom{d_v}{2} = \frac{1}{2}\sum_v \varepsilon_v(\varepsilon_v+1) \geq \sum_v \varepsilon_v = n-2$. Together with $\rho(X) \geq \sqrt{6}$ this gives the last claim. ∎

Theorem 3 of [4] states that K_n maximizes TSO among graphs of order n.

Remark. The statement is true. The proof in [4] consists of one sentence ("either there are fewer connected triples, or some vertices have degree less than $n-1$"), which is correct in spirit but does not show how the two effects combine. A complete argument is short and also covers disconnected graphs.

Proposition 5. *For $n \geq 3$, K_n is the unique maximizer of* TSO *among all graphs of order n.*

Proof. Each connected triple has $\rho \leq \sqrt{3}(n-1)$, and there are at most $\binom{n}{3}$ of them. Hence $\mathrm{TSO}(G) \leq \sqrt{3}(n-1)\binom{n}{3} = \mathrm{TSO}(K_n)$. Equality forces every 3-set to be connected and every degree to equal $n-1$, that is, $G = K_n$. ∎

Theorems 5 and 6 of [4] state that among trees of order n the star S_n has the largest TSO and the path P_n the smallest.

Remark. Theorem 5 of [4] is true (our Theorem 6 below), but its proof in [4] is not valid. It deletes a leaf v with neighbour u, sets $T' = T - v$, and asserts $\mathrm{TSO}(T) = \mathrm{TSO}(T') + \Delta_1 + (A - B)$, where Δ_1 collects the new wedges $(u; v, x)$ and $A - B$ the change in the wedges $(u; x, y)$ centred at u. This ignores that d_u also enters the wedges $(x; u, y)$ centred at the neighbours x of u. With $d = d_{T'}(u)$ and all other degrees taken in T', the correct identity is

$$\begin{aligned}\mathrm{TSO}(T) = \mathrm{TSO}(T') &+ \sum_{x\in N(u)} \sqrt{(d+1)^2 + 1 + d_x^2} \\ &+ \sum_{\{x,y\}\subseteq N(u)} \Big[\sqrt{d_x^2 + (d+1)^2 + d_y^2} - \sqrt{d_x^2 + d^2 + d_y^2}\Big] \\ &+ \sum_{x\in N(u)} \sum_{y\in N(x)\setminus\{u\}} \Big[\sqrt{d_x^2 + (d+1)^2 + d_y^2} - \sqrt{d_x^2 + d^2 + d_y^2}\Big],\end{aligned}$$

and the last sum is absent from [4]. It is positive, so the proof cannot be repaired by adding it: the inequality to be proved changes. We give a different proof below. The sums over $x, y \in N(u)$, $x \neq y$, in [4] are ambiguous: they may be read over unordered or over ordered pairs. We check both readings. Let $T' = P_5$ on vertices $1, \dots, 5$, and attach a new leaf v to $u = 2$ (so T is 2-methylpentane, with degree sequence $(3, 2, 2, 1, 1, 1)$ and $\mathrm{TSO}(T) \approx 17.923$). With unordered pairs the formula of [4] gives ≈ 17.264, and with ordered pairs ≈ 18.006; neither is correct. (For $T' = P_4$ and $u = 2$ the ordered reading happens to give the true value ≈ 14.542, so that smaller example does not refute the formula under both readings.) Over all trees T of order $4, \dots, 9$ and all leaves v of T (counted as labelled vertices, not up to automorphism), the formula of [4] fails in 372 of 405 cases with unordered pairs and in 401 of 405 cases with ordered pairs. (Here T' has $3, \dots, 8$ vertices, whereas in [4] it has n.) The same proof contains a second error: the bound $\Delta_1 \leq d\sqrt{n^2+2}$ is derived from the claim that the summand is increasing in d_x and so is largest when all neighbours are leaves, which contradicts the monotonicity. The bound itself holds: since $d_x + d \leq n$ for adjacent vertices of a tree on n vertices and $(d+1)^2 + d_x^2 + 1$ is convex, its maximum over $\{d + d_x \leq n,\ d, d_x \geq 1\}$ is attained at a vertex of this triangle and is at most $n^2 + 2$. But this is not the argument given.

Remark. Theorem 6 of [4] is also true (our Theorem 7 below). The argument in [4] (the path has the fewest connected triples, and the weight is increasing in each degree) does not compare the two effects: a tree with more triples may have smaller individual weights, and the number of triples and their weights cannot be minimized independently. The passage on the minimum of $\sum_v \binom{d_v}{2}$ in [4] (Lagrange multipliers, then "as equal as possible") is superseded by the identity $\sum_v \binom{d_v}{2} = \frac{1}{2}\sum_v \varepsilon_v(\varepsilon_v + 1) \geq n - 2$, where $\varepsilon_v = d_v - 1$, with equality if and only if all $\varepsilon_v \in \{0, 1\}$.

Lemma 3. *Let T be a tree of order $n \geq 3$ and $(v; a, b)$ a wedge of T. Then $d_v + d_a + d_b \leq n + 1$ and $d_v^2 + d_a^2 + d_b^2 \leq (n-1)^2 + 2$.*

Proof. The sets $\{a, v, b\}$, $N(a) \setminus \{v\}$, $N(b) \setminus \{v\}$, $N(v) \setminus \{a, b\}$ are pairwise disjoint, since a common element would close a cycle. Their sizes are 3,

$d_a - 1$, $d_b - 1$, $d_v - 2$, so $d_a + d_b + d_v - 1 \le n$. Put $x = d_v - 2$, $y = d_a - 1$, $z = d_b - 1$, so that $x, y, z \ge 0$ and $x + y + z \le n - 3 =: N$. Then

$$\begin{aligned} d_v^2 + d_a^2 + d_b^2 &= x^2 + y^2 + z^2 + 4x + 2y + 2z + 6 \\ &\le (x + y + z)^2 + 4(x + y + z) + 6 \\ &\le N^2 + 4N + 6 = (n - 1)^2 + 2. \end{aligned}$$

■

Theorem 6. *For every tree T of order $n \ge 3$,*

$$\mathrm{TSO}(T) \le \mathrm{TSO}(K_{1,n-1}) = \binom{n-1}{2}\sqrt{(n-1)^2 + 2},$$

with equality if and only if T is the star.

Proof. Put $\varepsilon_v = d_v - 1 \ge 0$, so $\sum_v \varepsilon_v = n - 2$. Then

$$\omega(T) = \frac{1}{2}\Big(\sum_v \varepsilon_v^2 + \sum_v \varepsilon_v\Big) \le \frac{1}{2}\big((n-2)^2 + (n-2)\big) = \binom{n-1}{2},$$

since $\sum \varepsilon_v^2 \le (\sum \varepsilon_v)^2$, with equality if and only if at most one ε_v is nonzero, that is, if and only if T is a star. By (2) and Lemma 3, each of the $\omega(T)$ terms of $\mathrm{TSO}(T)$ is at most $\sqrt{(n-1)^2 + 2}$. If T is not a star there are strictly fewer terms, and the inequality is strict. ■

Lemma 4. *Let T be a tree of order $n \ge 4$. Then $D_{\mathcal{T}}(T) \ge 6n - 14$, with equality if and only if $T = P_n$, and $D_{\mathcal{T}}(T) \ge 6n - 12$ if $T \ne P_n$.*

Proof. Let $\varepsilon_v = d_v - 1$ and $s_v = \sum_{a \sim v} d_a$. By (1) with $g(v) = d_v$,

$$D_{\mathcal{T}} = \sum_v \Big[d_v \binom{d_v}{2} + (d_v - 1)s_v\Big] = \sum_v \varepsilon_v \Big[\tfrac{1}{2}(\varepsilon_v + 1)^2 + s_v\Big],$$

and since $\sum_v \varepsilon_v = n - 2$,

$$D_{\mathcal{T}} - (6n - 12) = \sum_v \varepsilon_v \Big[\tfrac{1}{2}(\varepsilon_v + 1)^2 + s_v - 6\Big].$$

Leaves contribute 0. A vertex of degree 2 contributes $s_v - 4$, which is negative only if $s_v \le 3$. As $n \ge 4$, a vertex of degree 2 cannot have

two leaf neighbours, so $s_v = 3$, exactly one neighbour is a leaf, and the contribution is -1. Distinct such vertices have distinct leaf neighbours, so there are at most L of them, where $L = 2 + \sum_{d_v \geq 3}(d_v - 2)$ is the number of leaves. A vertex of degree $d \geq 3$ has $s_v \geq d$ and contributes at least $p(d) = (d-1)(\frac{1}{2}d^2 + d - 6)$; here $p(3) = 3$, $p(4) = 18$, and $p(d) - (d-2) \geq 2$ for $d \geq 3$. Let k be the number of vertices of degree at least 3. Then

$$D_{\mathcal{T}} - (6n-12) \geq -L + \sum_{d_v \geq 3} p(d_v) = -2 + \sum_{d_v \geq 3} \big(p(d_v) - (d_v - 2)\big) \geq -2 + 2k.$$

If $k = 0$ then $T = P_n$, and $D_{\mathcal{T}}(P_n) = 6n - 14$, because the two end triples have degree sum 5 and the remaining $n - 4$ have degree sum 6. If $k \geq 1$ then $D_{\mathcal{T}} \geq 6n - 12$. ∎

Theorem 7. *For every tree T of order $n \geq 4$,*

$$\mathrm{TSO}(T) \geq \mathrm{TSO}(P_n) = 6 + 2\sqrt{3}\,(n-4),$$

with equality if and only if $T = P_n$.

Proof. Let $T \neq P_n$. By Theorem 2(i) and Lemma 4,

$$\mathrm{TSO}(T) \geq \frac{D_{\mathcal{T}}(T)}{\sqrt{3}} \geq \frac{6n-12}{\sqrt{3}} = 2\sqrt{3}\,(n-2) = \mathrm{TSO}(P_n) + (4\sqrt{3} - 6),$$

and $4\sqrt{3} - 6 > 0.9$. ∎

Section 4 of [4] compares TSO with the Wiener index W, the Randić index χ, the Balaban index J and the Zagreb indices on the five isomers of C_6H_{14}.

Remark. The data in [4] contain several errors. In Table 5 of [4] the Wiener number of 2,2-dimethylbutane is 30 instead of 28. The Randić values are wrong for all five isomers; the value 2.914 listed as the Balaban index of *n*-hexane is its Randić index. In fact all five values of J in Table 5 of [4] (2.914, 3.104, 3.164, 3.164, 3.244) are wrong. The values of M_2 $(20, 22, 22, 24, 24)$ are wrong. The definition of J in [4] uses vertex degrees (with the usual prefactor $m/(\mu + 1)$, where μ is not defined in [4]), which

makes it a multiple of χ, whereas $J = \frac{m}{\mu+1}\sum_{uv\in E}(\sigma_u\sigma_v)^{-1/2}$ is defined through the distance sums $\sigma_u = \sum_x d(u,x)$ of the two end vertices of each edge uv, and $\mu = m-n+1$ is the cyclomatic number. Four of the five TSO values are off in the third decimal (17.924, 19.091, 31.061, 24.070 in place of 17.923, 19.090, 31.058, 24.069). Consequently the assertions that χ does not separate 2- and 3-methylpentane, that M_2 does not separate 2,2- and 2,3-dimethylbutane, and that J shows degeneracy, are false (Table 1): with the correct values χ, J and M_2 all separate the five isomers, so the rows for these three indices in Table 6 of [4] (which read 4/5, 4/5 and 3/5) should read 5/5. The coefficients in Table 8 of [4] (correlation with "branching", "compactness" and "symmetry") are undefined, cannot be obtained from five graphs, and are cited in the text as "Table 7"; the complexity column of Table 6 of [4] comes with no derivation.

Table 1. Values of TSO and of five classical indices for the isomers of C_6H_{14}.

isomer	TSO	W	χ	J	M_1	M_2
n-hexane	12.928	35	2.914	2.339	18	16
2-methylpentane	17.923	32	2.770	2.627	20	18
3-methylpentane	19.090	31	2.808	2.754	20	19
2,2-dimethylbutane	31.058	28	2.561	3.168	24	22
2,3-dimethylbutane	24.069	29	2.643	2.993	22	21

Proposition 8. *On the five isomers of* C_6H_{14} *the indices* TSO, W, χ, J, M_2 *take five distinct values, and* M_1 *takes four (it does not separate 2- and 3-methylpentane). For trees with* $\Delta \le 4$ *the numbers of distinct values are given in Table 2. In particular* TSO *is not injective on alkane trees: for* $a, b \ge 3$ *let* $Y(a,b,1)$ *be the tree formed by a vertex of degree* 3 *with three attached paths of lengths* $a, b, 1$. *Then*

$$\mathrm{TSO}(Y(a,b,1)) = 3\sqrt{17} + 2\sqrt{14} + 6 + 2\sqrt{3}\,(n-8), \qquad n = a+b+2,$$

so $Y(3,5,1)$ *and* $Y(4,4,1)$ *are non-isomorphic trees on ten vertices with the same* TSO.

Proof. The entries of Tables 1 and 2 come from direct enumeration (all

trees with $\Delta \le 4$ and $n \le 16$); two values were regarded as distinct if they differ by more than 10^{-9}. For the formula, the three wedges at the centre of $Y(a,b,1)$ have degree triples $(3;2,2)$, $(3;2,1)$, $(3;2,1)$, so $q = 17, 14, 14$. On a path of length $\ell \ge 3$ from the centre with vertices $v_1, \dots, v_\ell$ (v_ℓ a leaf), the wedge centred at v_1 has $q = 17$, those centred at $v_2, \dots, v_{\ell-2}$ have $q = 12$, and the one centred at $v_{\ell-1}$ has $q = 9$. Such a path therefore contributes $\sqrt{17} + 3 + (\ell - 3)\sqrt{12}$. Summing, the result depends only on $a + b$. ∎

Table 2. Number of distinct values of each index on all alkane trees with n carbon atoms (selected orders).

n	isomers	TSO	χ	J	W	M_2	M_1
8	18	18	16	18	16	13	6
9	35	35	28	35	16	16	7
10	75	73	49	75	40	21	8
12	355	315	137	349	87	28	10
14	1858	1412	350	1808	163	37	12
16	10359	6338	810	9923	276	45	14

Remark. Proposition 8 does not support the claim of [4] that TSO has superior discriminating power: four other indices separate the five isomers equally well. The claim of full discrimination is correct for the five isomers of C_6H_{14}, but it does not persist: already for $n = 10$ the index TSO takes only 73 values on the 75 alkane trees. Nor is the claim of a strong correlation with physicochemical properties supported, since [4] gives no data beyond five boiling points. For these five values the Pearson correlation coefficient is -0.97 for TSO, -0.98 for M_1, 0.97 for χ and 0.91 for W. Table 2 shows that for the orders listed ($n = 8, 9, 10, 12, 14, 16$) the index TSO separates more alkane trees than χ, W, M_1 and M_2, and for $n = 10, 12, 14, 16$ fewer than J (the two agree for $n = 8, 9$). We make no claim for other orders.

4 New results

The identity $\omega = \tau + 2t$ shows how triangles enter TSO. The following refinement of Theorem 2(i) measures the deviation from regularity.

Proposition 9. *If $\mathcal{T}(G) \neq \emptyset$, then*

$$\mathrm{TSO}(G) \geq \frac{D_{\mathcal{T}}}{\sqrt{3}} + \frac{1}{3+\sqrt{3}} \sum_{\{u,v,w\} \in \mathcal{T}(G)} \frac{(d_u - d_v)^2 + (d_v - d_w)^2 + (d_w - d_u)^2}{d_u + d_v + d_w},$$

with equality if and only if $d_u = d_v = d_w$ for every $\{u, v, w\} \in \mathcal{T}(G)$. For connected G of order at least 3 this holds if and only if G is regular (Theorem 2); in general, if and only if every component with at least three vertices is regular.

Proof. For a triple with degrees x, y, z put $S = x + y + z$ and $R = \sqrt{x^2 + y^2 + z^2}$, and

$$Q = (x-y)^2 + (y-z)^2 + (z-x)^2 = 3R^2 - S^2.$$

Then

$$R - \frac{S}{\sqrt{3}} = \frac{R^2 - S^2/3}{R + S/\sqrt{3}} = \frac{Q}{3(R + S/\sqrt{3})} \geq \frac{Q}{(3+\sqrt{3})S},$$

because $R \leq S$. Summing over $\mathcal{T}(G)$ gives the bound. Equality requires $Q = 0$ for every connected triple (the case $R = S$ would force two of the degrees to vanish). ∎

For regular graphs, Theorem 2(i) and Proposition 9 are equalities, and TSO can be computed exactly.

Theorem 10. *Let G be r-regular of order n. Then*

$$\mathrm{TSO}(G) = \sqrt{3}\, r \Big(\frac{nr(r-1)}{2} - 2t(G) \Big) = \frac{\sqrt{3}}{2}\, nr^2(r-1) - 2\sqrt{3}\, r\, t(G),$$

and, if $\lambda_1, \dots, \lambda_n$ are the adjacency eigenvalues of G,

$$\mathrm{TSO}(G) = \frac{\sqrt{3}}{2}\, nr^2(r-1) - \frac{\sqrt{3}\, r}{3} \sum_{i=1}^{n} \lambda_i^3.$$

If G is connected, then $\frac{\sqrt{3}}{6}\, nr^2(r-1) \le \mathrm{TSO}(G) \le \frac{\sqrt{3}}{2}\, nr^2(r-1)$; the right equality holds if and only if G is triangle-free, the left one if and only if $G = K_{r+1}$.

Proof. Each connected triple has weight $\sqrt{3}\, r$, and $\tau = \frac{nr(r-1)}{2} - 2t$ by Theorem 1; this gives the first formula. Since $\operatorname{tr} A^3 = 6t(G)$, we have $t = \frac{1}{6} \sum \lambda_i^3$, which yields the second.

Now let G be connected. The upper bound on TSO is $t \ge 0$, with equality if and only if G is triangle-free. For the lower bound note that a vertex lies in at most $\binom{r}{2}$ triangles and a triangle has three vertices, so $t \le nr(r-1)/6$. Substituting this into the first formula gives $\mathrm{TSO}(G) \ge \frac{\sqrt{3}}{6}\, nr^2(r-1)$. Equality in $t \le nr(r-1)/6$ holds if and only if the neighbourhood of every vertex is a clique, which for connected G means $G = K_{r+1}$. ∎

Corollary. *Let G_1, G_2 be r-regular graphs of the same order n. If $t(G_1) < t(G_2)$, then $\mathrm{TSO}(G_1) > \mathrm{TSO}(G_2)$; more precisely, $\mathrm{TSO}(G_1) - \mathrm{TSO}(G_2) = 2\sqrt{3}\, r\,(t(G_2) - t(G_1))$.*

Remark. Among regular graphs of fixed order and degree, each additional triangle lowers TSO by exactly $2\sqrt{3}\, r$. This sits uneasily with the description of TSO in [4] as capturing local clustering. For the two cubic graphs on six vertices, $\mathrm{TSO}(K_{3,3}) = 54\sqrt{3} \approx 93.53$ and $\mathrm{TSO}(\text{prism}) = 42\sqrt{3} \approx 72.75$. Note also that G is triangle-free if and only if $\sum \lambda_i^3 = 0$.

Proposition 11. *If G is r-regular and triangle-free, $r \ge 1$, then*

$$\mathrm{TSO}(G) = (r-1)\sqrt{\tfrac{3}{2}}\ \mathrm{SO}(G).$$

Proof. Here $\mathrm{SO}(G) = \frac{nr}{2} \cdot r\sqrt{2} = \frac{nr^2}{\sqrt{2}}$, while Theorem 10 with $t(G) = 0$ gives $\mathrm{TSO}(G) = \frac{\sqrt{3}}{2} nr^2(r-1)$. ∎

Theorem 12. *Let u, v be non-adjacent vertices of G. Then* $\mathrm{TSO}(G + uv) \geq \mathrm{TSO}(G)$*, with equality if and only if u and v are both isolated in G. In particular the inequality is strict if G is connected and $n \geq 3$.*

Proof. By Lemma 2, $\mathcal{T}(G) \subseteq \mathcal{T}(G + uv)$; degrees do not decrease, and the new triples contribute positive terms. Suppose u has a neighbour y. If $v \sim y$, then $\{u, v, y\}$ is connected in G and its weight increases strictly, since d_u increases. If $v \not\sim y$, then $\{u, v, y\}$ is connected in $G+uv$ but not in G, so $\mathcal{T}$ gains a member. The case where v has a neighbour is symmetric. If u and v are both isolated, no connected triple of G or $G + uv$ contains u or v, and nothing changes. ■

Proposition 13. *If G is a spanning subgraph of H, then* $\mathrm{TSO}(H) \geq \mathrm{TSO}(G)$*, with equality if and only if the edges of $H \setminus G$ form a matching on vertices that are isolated in G.*

Proof. Add the edges one at a time and apply Theorem 12. Equality throughout means that each added edge joins two vertices isolated at that moment. Since an endpoint ceases to be isolated, no vertex is used twice, and all these vertices were isolated in G. The converse is clear. ■

Theorem 14. *Let G be a connected graph of order $n \geq 4$. Then*

$$6 + 2\sqrt{3}\,(n-4) \leq \mathrm{TSO}(G) \leq \frac{\sqrt{3}}{6}\, n(n-1)^2(n-2),$$

with equality on the left if and only if $G = P_n$, and on the right if and only if $G = K_n$.

Proof. The right inequality is Proposition 5. For trees the left inequality is Theorem 7. If G is not a tree, it has a spanning tree $T \subsetneq G$. Adding the missing edges one at a time keeps the graph connected, so each step increases TSO strictly by Theorem 12, and $\mathrm{TSO}(G) > \mathrm{TSO}(T) \geq \mathrm{TSO}(P_n)$. ■

For the double star $\mathrm{DS}_{p,q}$, obtained by joining the centres of two stars with p and q leaves ($p, q \geq 1$), formula (2) gives

$$\mathrm{TSO}(\mathrm{DS}_{p,q}) = \binom{p}{2}\sqrt{(p+1)^2+2} + p\sqrt{(p+1)^2+(q+1)^2+1}$$

$$+\binom{q}{2}\sqrt{(q+1)^2+2}+q\sqrt{(q+1)^2+(p+1)^2+1}.$$

We now compare these results with Theorem 2 of [4], which gives, for connected G, the upper bound $\frac{\sqrt{3}}{2}n\Delta^2(\Delta-1)$ and the lower bounds $\frac{\sqrt{3}}{6}n\delta^2(\delta-1)$ for $\delta\geq 2$ and $(n-2)\sqrt{6}$ for $\delta=1$.

Proposition 15. *Let G be a connected graph of order $n\geq 4$. Then*

$$\mathrm{TSO}(G)\leq\sqrt{3}\,\Delta\Big(\frac{n\Delta(\Delta-1)}{2}-2t(G)\Big)\leq\frac{\sqrt{3}}{2}\,n\Delta^2(\Delta-1), \tag{3}$$

$$\mathrm{TSO}(G)\geq 6+2\sqrt{3}\,(n-4)>(n-2)\sqrt{6}, \tag{4}$$

$$\mathrm{TSO}(G)\geq\sqrt{3}\,\delta\,\tau(G)\geq\frac{\sqrt{3}}{6}\,n\delta^2(\delta-1)\quad(\delta\geq 2). \tag{5}$$

The first inequality in (3) *is strict unless G is Δ-regular, and the second is strict if G has a triangle. Equality holds in the first inequality of* (4) *only for $G=P_n$, and the last inequality of* (5) *is strict unless $G=K_n$. In particular, for $\delta=1$ the bound* (4) *is strictly stronger than $(n-2)\sqrt{6}$.*

Proof. Inequalities (3) and (5) are Proposition 4, and the first inequality of (4) is Theorem 14. For the strict inequality in (4) let $f(n)=6+2\sqrt{3}(n-4)-\sqrt{6}(n-2)$. Then $f(4)=6-2\sqrt{6}>0$ since $36>24$, and $f(n+1)-f(n)=2\sqrt{3}-\sqrt{6}>0$. ∎

Remark. In (3) the equality clause of the Remark in [4] becomes correct once the term $-2t(G)$ is retained: the first bound is attained exactly by the Δ-regular graphs, and the published bound only by those that are in addition triangle-free (for example C_5, where both equal $10\sqrt{3}$, but not K_4). The bounds $\mathrm{TSO}\leq\sqrt{\tau Q_\tau}\leq\sqrt{\Delta\tau D_\tau}$ of Theorem 2(ii) are given by exact invariants of G (Theorem 1); the second is attained exactly by the regular graphs, and the first by all regular graphs and also by stars (see the remark following Theorem 2). We do not compare it with (3) for general graphs.

Theorem 12 has a useful reformulation in terms of subgraphs, which is not in [4] and gives several lower bounds that do not involve δ. Note first

that TSO is additive over components and ignores isolated vertices, since a connected triple lies in one component and degrees do not change.

Theorem 16. *If H is a subgraph of G (not necessarily spanning or induced), then $\mathrm{TSO}(H) \le \mathrm{TSO}(G)$. If G is connected of order at least 3 and $H \neq G$, the inequality is strict. Moreover, if $H_1, \dots, H_s$ are pairwise vertex-disjoint subgraphs of G, then $\mathrm{TSO}(G) \ge \sum_{i=1}^{s} \mathrm{TSO}(H_i)$.*

Proof. Let H' be the graph obtained from H by adding the vertices of G not in H as isolated vertices. Then H' is a spanning subgraph of G and $\mathrm{TSO}(H') = \mathrm{TSO}(H)$, so the first claim is Proposition 13. Suppose G is connected, $n \ge 3$, and equality holds. By Proposition 13 the edges of $G \setminus H'$ form a matching M on vertices that are isolated in H'. An edge of M is then the only edge of G at each of its ends, so it would be a component of G isomorphic to K_2, which is impossible. Hence $M = \emptyset$ and G and H' have the same edges. As G has no isolated vertex, H' has none either, so $H' = H = G$. For the last claim, the graph $H_1 \cup \dots \cup H_s$ is a subgraph of G, and its TSO is the sum of the $\mathrm{TSO}(H_i)$. ∎

Corollary. *Let G be a connected graph of order $n \ge 3$.*

(a) $\mathrm{TSO}(G) \ge \binom{\Delta}{2}\sqrt{\Delta^2+2}$, *with equality if and only if $G = K_{1,\Delta}$.*

(b) If G contains a path on $p \ge 4$ vertices, then $\mathrm{TSO}(G) \ge 6 + 2\sqrt{3}\,(p-4)$, with equality if and only if $G = P_p$.

(c) If G contains a cycle of length $\ell \ge 4$, then $\mathrm{TSO}(G) \ge 2\sqrt{3}\,\ell$, with equality if and only if $G = C_\ell$. In particular, a Hamiltonian graph of order $n \ge 4$ satisfies $\mathrm{TSO}(G) \ge 2\sqrt{3}\,n$.

(d) If G contains a clique of order $\kappa \ge 3$, then $\mathrm{TSO}(G) \ge \frac{\sqrt{3}}{6}\,\kappa(\kappa-1)^2(\kappa-2)$, with equality if and only if $G = K_\kappa$.

(e) If $x_1, \dots, x_s$ are vertices whose closed neighbourhoods are pairwise disjoint, then $\mathrm{TSO}(G) \ge \sum_i \binom{d_{x_i}}{2}\sqrt{d_{x_i}^2+2}$.

Proof. Apply Theorem 16 to the subgraphs $K_{1,\Delta}$ (a vertex of maximum degree with its neighbours), P_p, C_ℓ, K_κ, and to the stars $K_{1,d_{x_i}}$ centred at the x_i, whose values come from Proposition 3. ∎

Remark. Part (a) improves on $6 + 2\sqrt{3}\,(n-4)$ as soon as the maximum degree is large compared with n (roughly $\Delta^3 \gtrsim 7n$), and (c) improves on

it by $8\sqrt{3} - 6 > 7.8$ for Hamiltonian graphs. For instance, $G = K_{3,3}$ is Hamiltonian and $\mathrm{TSO}(G) = 54\sqrt{3} \approx 93.5$, whereas the bound is $12\sqrt{3} \approx 20.8$; the bound is only sharp for the cycle itself. The point of the corollary is that the bounds depend on the structure of G and not on δ, which is 1 for most chemical trees.

For trees, Theorem 7 identifies the smallest value. The next value seems to be attained by a very specific tree. For $n \geq 6$ let F_n be the tree obtained from P_{n-1} by attaching a pendant vertex to the second vertex of the path; equivalently, the spider with legs of lengths $1, 1, n-3$. Counting wedges as in the proof of Proposition 8 gives $\mathrm{TSO}(F_n) = \sqrt{11} + 2\sqrt{14} + \sqrt{17} + 3 + 2\sqrt{3}\,(n-6)$. More generally, for $3 \leq \Delta \leq n-3$ let $F_{n,\Delta}$ be the spider with $\Delta - 1$ legs of length 1 and one leg of length $n - \Delta$; then

$$\mathrm{TSO}(F_{n,\Delta}) = \binom{\Delta - 1}{2}\sqrt{\Delta^2 + 2} + (\Delta - 1)\sqrt{\Delta^2 + 5} + \sqrt{\Delta^2 + 8} + 3 + 2\sqrt{3}\,(n - \Delta - 3).$$

5 Computational evidence and open problems

The following statements were found by computer search; they are not used elsewhere in the paper. The programs behind all computations reported in this paper (the enumerations in Section 3 and the searches below) are available from the authors on request.

Conjecture 1. *Among connected unicyclic graphs of order $n \geq 5$, the minimum of* TSO *is attained by the triangle with a pendant path attached at one vertex, the second smallest value is $\mathrm{TSO}(C_n) = 2\sqrt{3}\,n$, and the maximum is attained by the star plus one edge. (Verified for $5 \leq n \leq 12$, including uniqueness of the three extremal graphs.)*

Conjecture 2. *Among connected triangle-free graphs of order $n \geq 4$, the maximum of* TSO *is attained by $K_{\lfloor n/2 \rfloor, \lceil n/2 \rceil}$. (Verified for $n \leq 10$ by generating all triangle-free graphs of these orders, with $K_{\lfloor n/2 \rfloor, \lceil n/2 \rceil}$ the*

unique maximizer; among the graphs $K_{a,n-a}$ the balanced one is largest for $4 \le n \le 120$. Since TSO *is strictly increasing under edge addition, it suffices to consider maximal triangle-free graphs.)*

Conjecture 3. *Let T be a tree of order $n \ge 6$ with $T \ne P_n$. Then* $\mathrm{TSO}(T) \ge \mathrm{TSO}(F_n)$*, with equality if and only if $T = F_n$. More generally, if T has maximum degree Δ with $3 \le \Delta \le n-3$, then* $\mathrm{TSO}(T) \ge \mathrm{TSO}(F_{n,\Delta})$*. (Verified for all trees with $n \le 14$ in the first statement, and for $6 \le n \le 14$ and all $3 \le \Delta \le n-3$ in the second.) By Theorem 16, the second statement would imply* $\mathrm{TSO}(G) \ge \mathrm{TSO}(F_{n,\Delta})$ *for every connected graph G of order n and maximum degree Δ with $3 \le \Delta \le n-3$, because G has a spanning tree in which a vertex of maximum degree keeps all its neighbours.*

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