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The Sum of a Topological Index and Its Reciprocal Index

Wei Gao

Department of Mathematics, Pennsylvania State University at Abington, Abington, PA, 19001, USA

wvg5121@psu.edu

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Abstract

Let G be a simple connected graph. For a vertex-degree-based topological index $TI_f(G) = \sum_{uv \in E(G)} f(d_u, d_v)$, where $f(x, y)$ is a pertinently chosen symmetric real function, the topological index $RTI_f(G) = \sum_{uv \in E(G)} \frac{1}{f(d_u,d_v)}$ is called the reciprocal index of TI_f. In this paper, for the first Zagreb index ($f(x, y) = x + y$), the second Zagreb index ($f(x, y) = xy$), and the forgotten index ($f(x, y) = x^2 + y^2$), we prove that the star S_n and the path P_n achieve the maximum and minimum values of $TI_f + RTI_f$ among all trees of order n, respectively. In addition, we show that the same conclusion holds for some other vertex-degree-based topological indices.

1 Introduction

All graphs considered are assumed to be simple and connected. Let G be such a graph with vertex set $V(G)$ and edge set $E(G)$. The degree d_v of a vertex $v \in V(G)$ is the number of vertices adjacent to v in G. Let $\mathcal{T}_n$ be the set of all trees of order n. S_n and P_n denote the star and the path of order n, respectively.

A vertex-degree-based topological index (VDB topological index) of G is defined as

$$TI_f = TI_f(G) = \sum_{uv \in E(G)} f(d_u, d_v), \tag{1.1}$$

where $f(x, y)$ is a pertinently chosen symmetric real function with $x \geq 1$ and $y \geq 1$. The reciprocal index of TI_f is the topological index defined as

$$RTI_f = RTI_f(G) = \sum_{uv \in E(G)} \frac{1}{f(d_u, d_v)}. \tag{1.2}$$

Among the topological indices existing in the current literature, there are quite a few (TI_f, RTI_f)-pairs (see [5]). Recently, a number of papers appeared, concerned with the product of a topological index and its reciprocal [1, 3, 5, 6, 12–14].

In this paper, we are interested in the relations between TI_f and RTI_f, and especially in the properties of the sum $TI_f + RTI_f$. For the following three vertex-degree-based topological indices:

- First Zagreb index ($f(x, y) = x + y$) [8]:

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v);$$

- Second Zagreb index ($f(x, y) = xy$) [7]:

$$M_2(G) = \sum_{uv \in E(G)} d_u d_v;$$

- Forgotten index ($f(x, y) = x^2 + y^2$) [2]:

$$F(G) = \sum_{uv \in E(G)} (d_u^2 + d_v^2),$$

we prove that the star S_n uniquely maximizes $TI_f + RTI_f$ among all trees of order n, and the path P_n uniquely minimizes $TI_f + RTI_f$ among all trees of order n. In Section 4, we show that this result also holds for some other vertex-degree-based topological indices.

2 Some lemmas

Lemma 2.1. *Let $f(x,y)$ be one of the three functions $x+y$, xy, and x^2+y^2. Let $H(x,y,z) = f(x+z,y) + \frac{1}{f(x+z,y)} - f(x+1,y) - \frac{1}{f(x+1,y)}$ with $x \geq 1$, $y \geq 1$, and $z \geq 2$. Then the function $H(x,y,z)$ is strictly increasing on y.*

Proof. If $f(x,y) = x+y$, then

$$H(x,y,z) = \frac{1}{x+y+z} - \frac{1}{x+y+1} + z - 1.$$

So

$$\frac{\partial H(x,y,z)}{\partial y} = \frac{1}{(x+y+1)^2} - \frac{1}{(x+y+z)^2} > 0.$$

If $f(x,y) = xy$, then

$$H(x,y,z) = \frac{1}{xy+yz} - \frac{1}{xy+y} + y(z-1),$$

and

$$\frac{\partial H(x,y,z)}{\partial y} = \frac{1}{(x+1)y^2} - \frac{1}{(x+z)y^2} + z - 1 > 0.$$

If $f(x,y) = x^2+y^2$, then

$$H(x,y,z) = \frac{1}{(x+z)^2+y^2} - \frac{1}{(x+1)^2+y^2} + 2x(z-1) + z^2 - 1,$$

and

$$\frac{\partial H(x,y,z)}{\partial y} = \frac{2y}{\left((x+1)^2+y^2\right)^2} - \frac{2y}{\left((x+z)^2+y^2\right)^2} > 0.$$

The lemma holds. ■

Lemma 2.2. *Let $S_n \neq T \in \mathcal{T}_n$, and $e = uv \in E(T)$ be a non-pendent edge of T. Let T' be the tree obtained from T by deleting the edge uv, identifying u and v, and adding a new pendent vertex w adjacent to u. If*

$f(x,y)$ is one of the three functions $x+y$, xy, and x^2+y^2, then

$$TI_f(T)+RTI_f(T)<TI_f(T')+RTI_f(T').$$

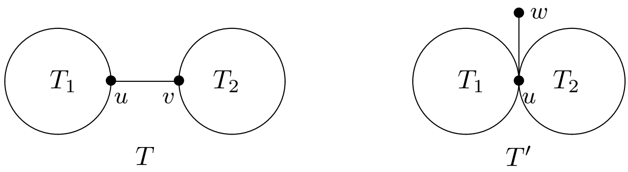

Figure 1. The trees T and T' in Lemma 2.2

Proof. Let $d_T(u)=s+1$, $d_T(v)=t+1$, $N_T(u)=\{v,u_1,\ldots,u_s\}$, and $N_T(v)=\{u,v_1,\ldots,v_t\}$. Then $s\geq 1$, $t\geq 1$,

$$\begin{aligned}&TI_f(T)-TI_f(T')\\=&\sum_{i=1}^{s}f(s+1,d_{u_i})+\sum_{j=1}^{t}f(t+1,d_{v_i})+f(s+1,t+1)\\&-\sum_{i=1}^{s}f(s+t+1,d_{u_i})-\sum_{j=1}^{t}f(s+t+1,d_{v_i})-f(s+t+1,1),\end{aligned}$$

and

$$\begin{aligned}&RTI_f(T)-RTI_f(T')\\=&\sum_{i=1}^{s}\frac{1}{f(s+1,d_{u_i})}+\sum_{j=1}^{t}\frac{1}{f(t+1,d_{v_i})}+\frac{1}{f(s+1,t+1)}\\&-\sum_{i=1}^{s}\frac{1}{f(s+t+1,d_{u_i})}-\sum_{j=1}^{t}\frac{1}{f(s+t+1,d_{v_i})}-\frac{1}{f(s+t+1,1)}.\end{aligned}$$

So

$$TI_f(T)+RTI_f(T)-\big(TI_f(T')+RTI_f(T')\big)$$

$$= \sum_{i=1}^{s} \left(f(s+1, d_{u_i}) + \frac{1}{f(s+1, d_{u_i})} - f(s+t+1, d_{u_i}) - \frac{1}{f(s+t+1, d_{u_i})} \right)$$
$$+ \sum_{j=1}^{t} \left(f(t+1, d_{v_j}) + \frac{1}{f(t+1, d_{v_j})} - f(s+t+1, d_{v_j}) - \frac{1}{f(s+t+1, d_{v_j})} \right)$$
$$+ f(s+1, t+1) + \frac{1}{f(s+1, t+1)} - f(s+t+1, 1) - \frac{1}{f(s+t+1, 1)}.$$

By Lemma 2.1,

$$TI_f(T) + RTI_f(T) - \big(TI_f(T') + RTI_f(T')\big)$$
$$\leq s \left(f(s+1, 1) + \frac{1}{f(s+1, 1)} - f(s+t+1, 1) - \frac{1}{f(s+t+1, 1)} \right)$$
$$+ t \left(f(t+1, 1) + \frac{1}{f(t+1, 1)} - f(s+t+1, 1) - \frac{1}{f(s+t+1, 1)} \right)$$
$$+ f(s+1, t+1) + \frac{1}{f(s+1, t+1)} - f(s+t+1, 1) - \frac{1}{f(s+t+1, 1)}$$
$$= sf(s+1, 1) + tf(t+1, 1) + f(s+1, t+1) + \frac{s}{f(s+1, 1)} + \frac{t}{f(t+1, 1)}$$
$$+ \frac{1}{f(s+1, t+1)} - (s+t+1)f(s+t+1, 1) - \frac{s+t+1}{f(s+t+1, 1)}$$
$$= \begin{cases} -\frac{st\left(2s^2t+4s^2+2st^2+12st+15s+4t^2+15t+12\right)}{(s+2)(t+2)(s+t+2)}, & \text{if } f(x,y) = x+y, \\ -\frac{st(st+s+t)}{(s+1)(t+1)}, & \text{if } f(x,y) = xy, \\ -\frac{st \cdot A}{\left(s^2+2s+2\right)\left(t^2+2t+2\right)\left(s^2+2s+t^2+2t+2\right)\left(s^2+2st+2s+t^2+2t+2\right)}, & \text{if } f(x,y) = x^2+y^2, \end{cases}$$

where

$$\begin{aligned} A = {} & 3s^7\left(t^2+2t+2\right) + s^6\left(9t^3+42t^2+66t+48\right) + s^5\left(12t^4+90t^3+246t^2\right. \\ & \left.+312t+179\right) + 2s^4\left(6t^5+54t^4+207t^3+408t^2+425t+201\right) \\ & + s^3\left(9t^6+90t^5+414t^4+1080t^3+1665t^2+1450t+580\right) \\ & + s^2\left(3t^7+42t^6+246t^5+816t^4+1665t^3+2118t^2+1566t+536\right) \\ & + 2s\left(3t^7+33t^6+156t^5+425t^4+725t^3+783t^2+496t+146\right) \\ & + 6t^7+48t^6+179t^5+402t^4+580t^3+536t^2+292t+72. \end{aligned}$$

Thus $TI_f(T) + RTI_f(T) < TI_f(T') + RTI_f(T')$. ■

Lemma 2.3. *Let $T_1 \in \mathcal{T}_n$ and $T_1' = T_1 - vv_2 + v_1v_2$ be trees depicted in Figure 2, where T_0 is a subtree of T_1 and $d_{T_1}(v) \geq 3$. Let $f(x,y)$ be one* *of the three functions $x+y$, xy, and x^2+y^2. Then*

$$TI_f(T_1)+RTI_f(T_1)>TI_f(T_1')+RTI_f(T_1').$$

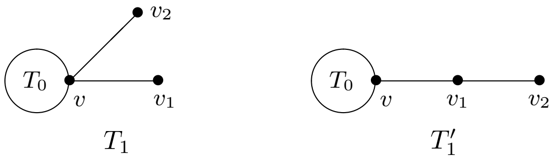

Figure 2. Trees T_1 and T_1' in Lemma 2.3

Proof. Let $d_{T_1}(v)=s+2$, and $N_{T_1}(v)=\{v_1,v_2,u_1,\ldots,u_s\}$. Then $s\geq 1$,

$$\begin{aligned}&TI_f(T_1)-TI_f(T_1')\\&=\sum_{i=1}^{s}f(s+2,d_{u_i})+2f(s+2,1)-\sum_{i=1}^{s}f(s+1,d_{u_i})-f(s+1,2)-f(2,1),\end{aligned}$$

and

$$\begin{aligned}&RTI_f(T_1)-RTI_f(T_1')\\&=\sum_{i=1}^{s}\frac{1}{f(s+2,d_{u_i})}+\frac{2}{f(s+2,1)}-\sum_{i=1}^{s}\frac{1}{f(s+1,d_{u_i})}-\frac{1}{f(s+1,2)}-\frac{1}{f(2,1)}.\end{aligned}$$

By Lemma 2.1,

$$\begin{aligned}&TI_f(T_1)+RTI_f(T_1)-\big(TI_f(T_1')+RTI_f(T_1')\big)\\&=\sum_{i=1}^{s}\left(f(s+2,d_{u_i})+\frac{1}{f(s+2,d_{u_i})}-f(s+1,d_{u_i})-\frac{1}{f(s+1,d_{u_i})}\right)\\&\quad+2f(s+2,1)+\frac{2}{f(s+2,1)}-f(s+1,2)-f(2,1)-\frac{1}{f(s+1,2)}-\frac{1}{f(2,1)}\\&\geq s\left(f(s+2,1)+\frac{1}{f(s+2,1)}-f(s+1,1)-\frac{1}{f(s+1,1)}\right)\\&\quad+2f(s+2,1)+\frac{2}{f(s+2,1)}-f(s+1,2)-f(2,1)-\frac{1}{f(s+1,2)}-\frac{1}{f(2,1)}\\&=(s+2)f(s+2,1)+\frac{s+2}{f(s+2,1)}-sf(s+1,1)-\frac{s}{f(s+1,1)}\end{aligned}$$

$$- f(s+1,2) - f(2,1) - \frac{1}{f(s+1,2)} - \frac{1}{f(2,1)}$$

$$= \begin{cases} \frac{s(6s^2+29s+31)}{3(s+2)(s+3)}, & \text{if } f(x,y) = x+y, \\ \frac{s(2s+1)}{2(s+1)}, & \text{if } f(x,y) = xy, \\ \frac{s(15s^7+165s^6+839s^5+2602s^4+5288s^3+6992s^2+5534s+2115)}{5(s^2+2s+2)(s^2+2s+5)(s^2+4s+5)}, & \text{if } f(x,y) = x^2+y^2. \end{cases}$$

So $TI_f(T) + RTI_f(T) > TI_f(T') + RTI_f(T')$. ■

Lemma 2.4. *Let $T_2 \in \mathcal{T}_n$ and $T_2' = T_2 - vv_{t+1} + v_t v_{t+1}$ be trees depicted in Figure 3, where T_0 is a subtree of T_2, $d_{T_2}(v) \geq 3$ and $t \geq 2$. Let $f(x,y)$ be one of the three functions $x+y$, xy, and x^2+y^2. Then*

$$TI_f(T_2) + RTI_f(T_2) > TI_f(T_2') + RTI_f(T_2').$$

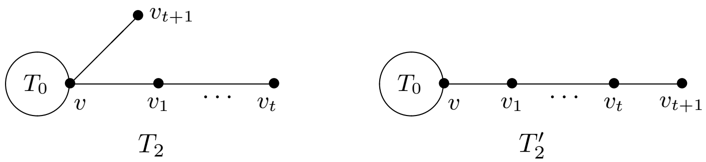

Figure 3. Trees T_2 and T_2' in Lemma 2.4

Proof. Let $d_{T_2}(v) = s+2$, and $N_{T_2}(v) = \{v_1, v_{t+1}, u_1, \ldots, u_s\}$. Then $s \geq 1$,

$$TI_f(T_2) - TI_f(T_2') = \sum_{i=1}^{s} f(s+2, d_{u_i}) + f(s+2,2) + f(s+2,1) - \sum_{i=1}^{s} f(s+1, d_{u_i}) - f(s+1,2) - f(2,2),$$

and

$$RTI_f(T_2) - RTI_f(T_2') = \sum_{i=1}^{s} \frac{1}{f(s+2, d_{u_i})} + \frac{1}{f(s+2,2)} + \frac{1}{f(s+2,1)} - \sum_{i=1}^{s} \frac{1}{f(s+1, d_{u_i})} - \frac{1}{f(s+1,2)} - \frac{1}{f(2,2)}.$$

So by Lemma 2.1,

$$\begin{aligned}
&TI_f(T_2)+RTI_f(T_2)-(TI_f(T_2')+RTI_f(T_2'))\\
=&\sum_{i=1}^{s}\left(f(s+2,d_{u_i})+\frac{1}{f(s+2,d_{u_i})}-f(s+1,d_{u_i})-\frac{1}{f(s+1,d_{u_i})}\right)\\
&+f(s+2,2)+f(s+2,1)+\frac{1}{f(s+2,2)}+\frac{1}{f(s+2,1)}\\
&-f(s+1,2)-f(2,2)-\frac{1}{f(s+1,2)}-\frac{1}{f(2,2)}\\
\geq\ & s\left(f(s+2,1)+\frac{1}{f(s+2,1)}-f(s+1,1)-\frac{1}{f(s+1,1)}\right)\\
&+f(s+2,2)+f(s+2,1)+\frac{1}{f(s+2,2)}+\frac{1}{f(s+2,1)}\\
&-f(s+1,2)-f(2,2)-\frac{1}{f(s+1,2)}-\frac{1}{f(2,2)}\\
=&\begin{cases}\frac{8s^4+71s^3+199s^2+170s}{4(s+2)(s+3)(s+4)}, & \text{if } f(x,y)=x+y,\\ \frac{8s^3+23s^2+13s}{4(s+1)(s+2)}, & \text{if } f(x,y)=xy,\\ \frac{B}{8(s^2+2s+2)(s^2+2s+5)(s^2+4s+5)(s^2+4s+8)}, & \text{if } f(x,y)=x^2+y^2,\end{cases}
\end{aligned}$$

where

$$\begin{aligned}
B=&\ 24s^{10}+360s^9+2591s^8+11652s^7+35896s^6+78498s^5\\
&+121679s^4+128934s^3+84982s^2+27384s.
\end{aligned}$$

Thus $TI_f(T_2)+RTI_f(T_2)>TI_f(T_2')+RTI_f(T_2')$. ■

Lemma 2.5. *Let $T_3\in\mathcal{T}_n$ and $T_3'=T_3-vw_1+v_tw_1$ be trees depicted in Figure 4, where T_0 as a subtree of T_3, $d_{T_3}(v)\geq 3$, $r\geq 2$, and $t\geq 2$. Let $f(x,y)$ be one of the three functions $x+y$, xy, and x^2+y^2. Then*

$$TI_f(T_3)+RTI_f(T_3)>TI_f(T_3')+RTI_f(T_3').$$

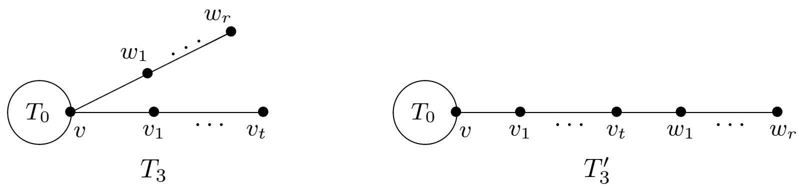

Figure 4. Trees T_3 and T_3' in Lemma 2.5

Proof. Let $d_{T_3}(v) = s+2$, and $N_{T_3}(v) = \{v_1, w_1, u_1, \ldots, u_s\}$. Then $s \geq 1$,

$$TI_f(T_3) - TI_f(T_3') = \sum_{i=1}^{s} f(s+2, d_{u_i}) + 2f(s+2,2) + f(2,1) - \sum_{i=1}^{s} f(s+1, d_{u_i}) - f(s+1,2) - 2f(2,2),$$

and

$$RTI_f(T_3) - RTI_f(T_3') = \sum_{i=1}^{s} \frac{1}{f(s+2, d_{u_i})} + \frac{2}{f(s+2,2)} + \frac{1}{f(2,1)} - \sum_{i=1}^{s} \frac{1}{f(s+1, d_{u_i})} - \frac{1}{f(s+1,2)} - \frac{2}{f(2,2)}.$$

By Lemma 2.1,

$$\begin{aligned}
&TI_f(T_3) + RTI_f(T_3) - (TI_f(T_3') + RTI_f(T_3')) \\
&= \sum_{i=1}^{s} \left(f(s+2, d_{u_i}) + \frac{1}{f(s+2, d_{u_i})} - f(s+1, d_{u_i}) - \frac{1}{f(s+1, d_{u_i})} \right) \\
&\quad + 2f(s+2,2) + f(2,1) + \frac{2}{f(s+2,2)} + \frac{1}{f(2,1)} \\
&\quad - f(s+1,2) - 2f(2,2) - \frac{1}{f(s+1,2)} - \frac{2}{f(2,2)} \\
&\geq s \left(f(s+2,1) + \frac{1}{f(s+2,1)} - f(s+1,1) - \frac{1}{f(s+1,1)} \right) \\
&\quad + 2f(s+2,2) + f(2,1) + \frac{2}{f(s+2,2)} + \frac{1}{f(2,1)}
\end{aligned}$$

$$- f(s+1,2) - 2f(2,2) - \frac{1}{f(s+1,2)} - \frac{2}{f(2,2)}$$

$$= \begin{cases} \frac{12s^4+107s^3+303s^2+262s}{6(s+2)(s+3)(s+4)}, & \text{if } f(x,y) = x+y, \\ \frac{6s^3+18s^2+11s}{2(s+1)(s+2)}, & \text{if } f(x,y) = xy, \\ \frac{C}{20(s^2+2s+2)(s^2+2s+5)(s^2+4s+5)(s^2+4s+8)}, & \text{if } f(x,y) = x^2+y^2, \end{cases}$$

where

$$C = 60s^{10} + 900s^9 + 6479s^8 + 29148s^7 + 89848s^6 + 196650s^5 + 305171s^4 + 323922s^3 + 213982s^2 + 69240s.$$

So $TI_f(T_3) + RTI_f(T_3) > TI_f(T_3') + RTI_f(T_3')$. ■

3 Main result

Theorem 3.1. *Let $f(x,y)$ be one of the three functions $x+y$, xy, and x^2+y^2. Then for any $T \in \mathcal{T}_n$,*

$$TI_f(P_n) + RTI_f(P_n) \leq TI_f(T) + RTI_f(T) \leq TI_f(S_n) + RTI_f(S_n).$$

The left equality holds if and only if $T \cong P_n$, and the right equality holds if and only if $T \cong S_n$.

Proof. Let $T \in \mathcal{T}_n$. If $T \neq S_n$, then T has at least one non-pendent edge. By Lemma 2.2, there is a tree $T' \in \mathcal{T}_n$ such that $TI_f(T) + RTI_f(T) < TI_f(T') + RTI_f(T')$. Thus the upper bound holds.

If $T \neq P_n$, then by Lemmas 2.3, 2.4 and 2.5, there is a tree $T' \in \mathcal{T}_n$ such that $TI_f(T) + RTI_f(T) > TI_f(T') + RTI_f(T')$. The lower bound holds. ■

4 Conclusions

In this paper, for three vertex-degree-based topological indices (first Zagreb index, second Zagreb index, forgotten index), we show that the star S_n and the path P_n achieve the maximum and minimum values of

$TI_f + RTI_f$ among all trees of order n, respectively.

It can be verified that Lemmas 2.2, 2.3, 2.4 and 2.5 also hold for some other vertex-degree-based topological indices. For example,

- First hyper-Zagreb index ($f(x,y) = (x+y)^2$) [15]:

$$HM_1(G) = \sum_{uv \in E(G)} (d_u + d_v)^2;$$

- First Gourava index ($f(x,y) = x + y + xy$) [10]:

$$GO_1(G) = \sum_{uv \in E(G)} (d_u + d_v + d_u d_v);$$

- Second Gourava index ($f(x,y) = (x+y)xy$) [10]:

$$GO_2(G) = \sum_{uv \in E(G)} (d_u + d_v) d_u d_v;$$

- Reciprocal Randić index ($f(x,y) = \sqrt{xy}$) [4]:

$$RR(G) = \sum_{uv \in E(G)} \sqrt{d_u d_v};$$

- First K Banhatti index ($f(x,y) = [x + (x+y-2)] + [y + (x+y-2)]$) [9,11]:

$$B_1(G) = \sum_{uv \in E(G)} [[d_u + (d_u + d_v - 2)] + [d_v + (d_u + d_v - 2)]];$$

- Second K Banhatti index ($f(x,y) = x(x+y-2) + y(x+y-2)$) [9,11]:

$$B_2(G) = \sum_{uv \in E(G)} [d_u(d_u + d_v - 2) + d_v(d_u + d_v - 2)].$$

So for each of the topological indices TI_f above, by Theorem 3.1, the star S_n uniquely maximizes $TI_f + RTI_f$ over $\mathcal{T}_n$, and the path P_n uniquely minimizes $TI_f + RTI_f$ over $\mathcal{T}_n$.

Note that for each topological index mentioned in this article, the star S_n and path P_n reach their maximum and minimum values among all trees of $\mathcal{T}_n$, respectively. For their reciprocal indies, the results are just the opposite. So we believe that the following conjecture is true.

Conjecture 4.1. *If* $TI_f(P_n) \leq TI_f(T) \leq TI_f(S_n)$ *and* $RTI_f(S_n) \leq RTI_f(T) \leq RTI_f(P_n)$ *for any* $T \in \mathcal{T}_n$*, then*

$$TI_f(P_n) + RTI_f(P_n) \leq TI_f(T) + RTI_f(T) \leq TI_f(S_n) + RTI_f(S_n).$$

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