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On the Mostar Index of Trees and Product Graphs

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Abstract. If *G* is a graph, and if for $e = uv \in E(G)$ the number of vertices closer to *u* than to *v* is denoted by n_u , then $Mo(G) = \sum_{uv \in E(G)} |n_u - n_v|$ is the Mostar index of *G*. In this paper, the Mostar index is studied on trees and graph products. Lower and upper bounds are given on the difference between the Mostar indices of a tree and a tree obtained by contraction one of its edges and the corresponding extremal trees are characterized. An upper bound on the Mostar index for the class of all trees but the stars is proved. Extremal trees are also determined on the (k + 1)-th largest/smallest Mostar index. The index is also studied on Cartesian and corona products.

1. Introduction

If G = (V(G), E(G)) is a graph and $uv \in E(G)$, then the number of vertices that are closer (w.r.t. the standard shortest path metric) to u than to v is denoted by n_u ; analogously n_v is defined. With this notation in hand, the *Mostar index* of G is

$$\operatorname{Mo}(G) = \sum_{uv \in E(G)} |n_u - n_v|.$$

Denoting by $\phi_G(e) = |n_u - n_v|$ the contribution of the edge e = uv to Mo(*G*), we can write the Mostar index of *G* in an even more compact form as follows:

$$\operatorname{Mo}(G) = \sum_{e \in E(G)} \phi_G(e) \,.$$

The Mostar index received a lot of attention right away after its introduction in 2018 by Došlić et al. [12]. First, it was considered on several classes of chemically important graphs [4, 9, 14, 19]. The difference between the Mostar index and the irregularity of graphs was studied in [13]. Cacti and and extremal

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bicyclic graphs with respect to the Mostar index were studied in [17, 26], respectively. In [8], the Mostar index of diameter 2 graphs and of some graph operations was clarified. The paper [14] studies the Mostar index with respect to graph symmetries and describes the structures of graphs whose Mostar index is 1. Papers [10, 18] and [11] deal with the extremal values of the Mostar index of trees with different parameters and chemical trees, respectively. Finally, maximal Mostar indices in hexagonal chains were investigated in [27].

The Mostar index is naturally related to several established graph theory concepts. Let *G* be a graph. *G* is *distance-balanced* [20] if $\phi_G(e) = 0$ holds for each edge *e* of *G*, so that Mo(*G*) = 0 if and only if *G* is distance-balanced. The *irregularity* [3] of *G* is $irr(G) = \sum_{uv \in E(G)} |\deg(u) - \deg(v)|$, which was extended [1] to its total version $irr_t(G) = \sum_{\{u,v\} \subseteq V(G)} |\deg(u) - \deg(v)|$ called *total irregularity*. Some related results can be found in [28].

In this paper, some further results are obtained on the Mostar index of graphs. In Section 2, additional concepts and notation needed are given, and results to be used in later sections recalled. In Section 3 we consider the Mostar index of trees. We first give sharp lower and upper bounds on the difference between the Mostar indices of a tree and a tree obtained by contraction one of its edges. We follow with a general upper bound on the Mostar index for the class of all non-star trees, and give extremal trees on the (k + 1)-th largest/smallest Mostar index. In the final section we give a short proof of the formula for the Mostar index on Cartesian products and prove an exact result for corona products.

2. Preliminaries

Graphs considered in this paper are connected, unless stated otherwise. We use the notation $[n] = \{1, ..., n\}$ for $n \in \mathbb{N}$. If G = (V(G), E(G)) is a graph, then we denote by $N_G(v)$ the neighborhood of the vertex v of G. The size of N(v) is called the degree of v and denoted by $\deg_G(v)$ or simply $\deg(v)$. The order and the size of G will be denoted by n(G) and m(G), respectively. A vertex with $\deg(v) = 1$ is a *pendant vertex* (or *leaf* if G is a tree) in a graph G. If $e \in E(G)$, then G.e denotes the graph obtained from G by contracting the edge e. The *transmission* $\operatorname{Tr}_G(v)$ or simply $\operatorname{Tr}(v)$ of a vertex $v \in V(G)$ is the sum of the distances from v to all other vertices of G. The relevance of the transmission for the Mostar index follows from the following basic, important result.

Lemma 2.1. ([6]) If $uv \in E(G)$, then $Tr(u) - Tr(v) = n_v - n_u$.

Lemma 2.1 immediately yields:

Corollary 2.2. If G is a graph, then $Mo(G) = \sum_{uv \in E(G)} |Tr(u) - Tr(v)|$.

We note in passing that the right-hand side of the equality in Corollary 2.2 was introduced and studied in [25] under the name *transmission irregularity*.

Recall that $\phi_G(e) = |n_u - n_v|$ is the contribution of the edge e = uv to Mo(*G*). Hence it makes sense to say that *e* is *equi-effective* if $\phi_G(e) = 0$. We can then state that *G* is distance-balanced if and only if every edge of *G* is equi-effective.

To conclude the preliminaries, we recall the following result.

Proposition 2.3. ([12]) Let G be a graph of order n > 2 with $uv \in E(G)$. Then $|n_v - n_u| \le n - 2$ with equality if and only if one of u and v is a pendant vertex.

3. On the Mostar index of trees

In this section, we first consider the effect of edge contraction in trees on the Mostar index of trees, and follow with several extremal results on the Mostar index of trees. We begin with the following result that clearly holds by the structure of trees.

Lemma 3.1. Let T be a tree of order $n \ge 2$. Then T has at most one equi-effective edge. Moreover, if T has one equi-effective edge, then n is even.

If *T* is a tree and $v \in V(T)$, then let $\ell_T(v)$ denote the number of leaves adjacent to *v*. Our first main result now reads as follows.

Theorem 3.2. Let T be a tree with $n(T) = n \ge 3$, and let $e = uv \in E(T)$ with $s = \deg_T(u) \ge \deg_T(v)$. Then

$$n-2 \le \operatorname{Mo}(T) - \operatorname{Mo}(T.e) \le 2(n-2).$$

The left equality holds if and only if e is the equi-effective edge of T. The right equality is achieved if v is a leaf in T with

$$p = \ell_T(u) \ge \begin{cases} \max\{\max_{\substack{[i,j] \le [s-p]}} |n_u^{(i)} - n_u^{(j)}|, 1\}; & s-p \ge 2, \\ \max\{n_u^{(i)}, 1\}; & s-p = 1, \end{cases}$$

such that $T - u = \bigcup_{i=1}^{s-p} T_u^{(i)} \cup pK_1$ where $T_u^{(i)}$ is a non-trivial subtree of T - u of order $n_u^{(i)}$ for $i \in [s - p]$.

Proof. Let $T - e = T_u \cup T_v$ where T_u and T_v are components containing u and v, respectively. Assume that $n(T_u) \ge n(T_v)$. For any edge $f \in E(T_v)$, we have $\phi_T(f) = \phi_{T,e}(f) + 1$. Now we consider any edge $f = xy \in E(T_u)$. Let $T - f = T_x \cup T_y$ with d(x, u) < d(y, u). If $n(T_y) < n(T_x)$, we have $\phi_T(f) = \phi_{T,e}(f) + 1$ and while $n(T_y) \ge n(T_x)$, then $\phi_T(f) = \phi_{T,e}(f) - 1$ holds possibly. Assume that there are q edges f such that $\phi_T(f) - \phi_{T,e}(f) = 1$. Setting A = Mo(T) - Mo(T.e), we have

$$A = \phi_T(e) + \sum_{f \in E(T_v)} (\phi_T(f) - \phi_{T,e}(f)) + \sum_{f \in E(T_u)} (\phi_T(f) - \phi_{T,e}(f))$$

= $[n(T_u) - n(T_v)] + n(T_v) - 1 - q + [n(T_u) - 1 - q]$
= $2n(T_u) - 2 - 2q$
 $\leq 2(n-2)$

with equality holding if and only if $n(T_u) = n - 1$ and q = 0, that is, $\deg_T(v) = 1$ with q = 0. Next we characterize the structure of T with q = 0. First assume that $\deg_T(u) = s \ge p + 2$ and u has s - p non-leaf neighbors $u_i \in V(T_u^{(i)})$ in T for $i \in [s - p]$. Without loss of generality, we can assume that $\max_{\{i,j\} \subseteq [s-p]} |n_u^{(i)} - n_u^{(j)}| = 1$

 $n_u^{(1)} - n_u^{(2)}$. Note that $n = \sum_{i=1}^{s-p} n_u^{(i)} + p + 1$. In view of $p \ge \max\{\max_{\{i,j\} \subseteq [s-p]} |n_u^{(i)} - n_u^{(j)}|, 1\}$, we have $n_u^{(2)} \le n_u^{(1)} \le \frac{n-2}{2}$. Considering the contribution of uu_1 to Mo(*T*) and Mo(*T.e*), respectively, we have

$$\begin{split} \phi_T(uu_1) &= |n_u^{(1)} - (n - n_u^{(1)})| \\ &= n - 2n_u^{(1)} \\ &= |n_u^{(1)} - (n - 1 - n_u^{(1)})| + 1 \\ &= \phi_{T.e}(xy) + 1 \,. \end{split}$$

Analogously, $\phi_T(uu_i) = \phi_{T,e}(uu_i) + 1$ for any $i \in [s - p] \setminus \{1\}$. Now we choose any edge $xy \in E(T_u^{(1)})$ with d(x, u) < d(y, u). Recall that $n_u^{(1)} \le \frac{n-2}{2}$, we have

$$\phi_T(xy) = |n_x - (n - n_x)| = n - 2n_x = |n_x - (n - 1 - n_x)| + 1 = \phi_{T,e}(xy) + 1.$$

Moreover, we obtain $\phi_T(xy) = \phi_{T,e}(xy) + 1$ in a parallel way for any edge $xy \in E(T_u^{(i)})$ with $i \in [s-p] \setminus \{1\}$. By Proposition 2.3, for any pendant edge $f \neq e$ incident with u, we have $\phi_{T,e}(f) = n - 3 = n - 2 - 1 = \phi_T(f) - 1$. Recall that e = uv is a pendant edge in T. Then it follows that Mo(T) = Mo(T.e) + 2(n-2) as desired. For the case $\deg_T(u) = s = p + 1$, the result can be similarly proved and here we omit its proof.

Note that there are at most $\lfloor \frac{n(T_u)-n(T_v)}{2} \rfloor$ edges f = xy such that $n(T_y) \ge n(T_x)$, that is, $q \le \lfloor \frac{n(T_u)-n(T_v)}{2} \rfloor$. Then, from $n(T_u) + n(T_v) = n$, it follows that

$$Mo(T) - Mo(T.e) = 2n(T_u) - 2 - 2q$$

$$\geq 2n(T_u) - 2 - 2\left\lfloor \frac{n(T_u) - n(T_v)}{2} \right\rfloor$$

$$= n - 2$$

with equality holding if and only if $n(T_u) = n(T_v)$, that is, *e* is the equi-effective edge of *T*. Moreover, by Lemma 3.1, we conclude that *n* is even. This finishes the proof of the theorem. \Box

For the star S_n with $n \ge 2$, we have $Mo(S_n) - Mo(S_n.e) = 2(n-2)$ for any edge $e \in E(S_n)$. This is just the case s = p in the proof of Theorem 3.2.

Corollary 3.3. If T is a tree with $n(T) = n \ge 3$ and H is a proper subtree of T, then Mo(T) > Mo(H) + n - 2.

Proof. We prove the result by induction on the order of *T*. The statement holds for n = 3. Let e = uv be a pendant edge of *T* such that $e \notin E(H)$. By Theorem 3.2, we have Mo(T) > Mo(T.e) + n - 2, since *e* is never an equi-effective edge in *T*. Note that *H* is a subtree of *T.e.* Then, by induction hypothesis, we get $Mo(H) \le Mo(T.e)$. This completes the proof of the corollary. \Box

In [12] it was proved that $Mo(T) \le (n-1)(n-2)$ for any tree T with $n(T) = n \ge 4$ with equality holding if and only if T is a star. We next improve this result by giving an exact upper bound for all non-star trees. To prove the result, we need the following lemma.

Lemma 3.4. Let uv be a non-pendant edge in a tree of order $n \ge 4$. Then $|n_u - n_v| \le n - 4$ with equality holding if and only if either u or v is adjacent to a leaf of T.

Proof. Without loss of generality, we assume that $\deg_T(u) \ge \deg_T(v)$. Since uv is a non-pendant edge of *T*, we have $\deg_T(v) \ge 2$. By Proposition 2.3, $|n_u - n_v| < n - 2$ for uv being non-pendant in *T*. Note that $n_u + n_v = n$ in *T*. Then we have $|n_u - n_v| \le n - 4$ with equality holding if and only if $\max\{n_u, n_v\} = n - 2$ and $\min\{n_u, n_v\} = 2$. Equivalently, $\deg_T(v) = 2$ with v being adjacent to a leaf of *T*, completing the proof of the lemma. \Box

A *double star* $S_n(p,q)$ is a tree obtained from attaching $p \ge 1$ vertices to an end-vertex of K_2 and attaching n - p - 2 vertices to the other vertex of it where $0 \le p \le \lfloor \frac{n-2}{2} \rfloor$. Note that $S_n(0, n - 2)$ is the star graph S_n .

Theorem 3.5. Let T be a tree of order $n \ge 3$ different from S_n . Then we have $Mo(T) \le (n-1)(n-2) - 2$ with equality holding if and only if $T \ge S_n(1, n-3)$.

Proof. Let $T \not\cong S_n$ be a tree of order $n \ge 3$ with the maximum Mostar index. Since $T \not\cong S_n$, there is a non-pendant edge uv in T. Assume that $\deg_T(v) \le \deg_T(u)$. From Lemma 3.4 and Proposition 2.3, we have

$$Mo(T) = \phi_T(uv) + \sum_{e \in E(T) \setminus \{uv\}} \phi_T(e)$$

$$\leq n - 4 + (n - 2)^2$$

$$= (n - 1)(n - 2) - 2$$

with equality holding if and only if $\deg_T(v) = 2$ with v being adjacent to a leaf in T and other n - 2 edges are pendant in T, that is, $T \cong S_n(1, n - 3)$, finishing the proof of the theorem. \Box

Let $T_n(1, k, \ell)$ be a tree of order $n = k + \ell + 2$ obtained by attaching a pendant vertex at the vertex v_k of a path $P_{k+\ell+1} = v_0v_1v_2 \dots v_{k+\ell}v_{k+\ell}$ with natural adjacency relation where $k \in [\ell]$. To obtain the final result in this section, we first list a lemma and prove a preliminary result.

Lemma 3.6. ([12]) If T is a tree of order $n \ge 4$, then

$$\left\lfloor \frac{(n-1)^2}{2} \right\rfloor \le \operatorname{Mo}(T) \le (n-1)(n-2)$$

with left equality if and only if $T \cong P_n$ and right equality if and only if $T \cong S_n$.

Lemma 3.7. Let T be a tree. Then Mo(T) is an even number.

Proof. Let $n \ge 2$ be the order of T with $e = uv \in E(T)$. If $n_u = m$, then $|n_u - n_v| = |n - 2m|$. It means that the contribution of all edges to Mo(T) have the same parity. If n is even (odd, resp.), then Mo(T) is the sum of n - 1 even (odd, resp.) numbers. This implies that Mo(T) is an even number. \Box

Theorem 3.8. Among the trees of order $n \ge 4$, the (k + 1)-th largest Mostar index is attained at $S_n(k, n - 2 - k)$ with $1 \le k \le \lfloor \frac{n-2}{2} \rfloor$, and the (k + 1)-th smallest Mostar index is attained at $T_n(1, k, n - 2 - k)$ with $1 \le k \le \lfloor \frac{n-1}{2} \rfloor$.

Proof. From the definitions of the Mostar index and the double star $S_n(k, n-2-k)$, we have $Mo(S_n(k, n-2-k)) = (n-2)^2 + n - 2(k+1)$. Note that $Mo(S_n(k, n-2-k)) - Mo(S_n(k+1, n-3-k)) = 2$. Combining Theorem 3.5 with Lemmas 3.7 and 3.6, we conclude that the (k + 1)-th largest Mostar index is attained at $S_n(k, n-2-k)$ with $1 \le k \le \lfloor \frac{n-2}{2} \rfloor$.

From the structure of $T_n(1, k, n-2-k)$ and some elementary calculation, we have $Mo(T_n(1, k, n-2-k)) = \lfloor \frac{(n-1)^2}{2} \rfloor + 2k$ for every k with $1 \le k \le \lfloor \frac{n-1}{2} \rfloor$. By Lemmas 3.7 and 3.6, we have the result with the (k + 1)-th smallest Mostar index for $1 \le k \le \lfloor \frac{n-1}{2} \rfloor$. \Box

4. On the Mostar index of graph products

In [8] the Mostar index was considered on the join of graphs, the disjunction of graphs, and the symmetric difference of graphs. Graphs obtained by each of these operations have diameter at most 2, and for the latter graphs it was proved in [8] that their Mostar index equals the irregularity. We restate here this result and show that Corollary 2.2 enables a short simple proof of it.

Theorem 4.1. If G is a graph of diameter at most 2, then Mo(G) = irr(G).

Proof. The result is clear for complete graphs, hence let *G* be a graph with diameter 2. Then $\text{Tr}(u) = \deg_G(u) + 2[n - 1 - \deg_G(u)] = 2n - 2 - \deg_G(u)$ for any vertex $u \in V(G)$. Thus $\phi_G(uv) = |\deg_G(u) - \deg_G(v)|$ for every edge $uv \in E(G)$. The result now follows from Corollary 2.2. \Box

The Mostar index of graph products was further investigated in [2], where corona products, Cartesian products, joins of graphs, lexicographic products, and the so-called Indu-Bala products are treated. In this section we give some further insight in this direction. We first give a short proof of the formula for the Mostar index of Cartesian products and then give an exact result for the corona product.

4.1. Cartesian product

The Cartesian product $G_1 \square G_2$ of graphs G_1 and G_2 is the graph with the vertex set $V(G_1) \times V(G_2)$ and the edge set $\{(u_1, u_2)(v_1, v_2) : u_1 = v_1 \text{ and } u_2v_2 \in E(G_2), \text{ or } u_2 = v_2 \text{ and } u_1v_1 \in E(G_1)\}$. In [12] formulas were proved for the Mostar index of Cartesian products in which both factors are paths or both factors are partial cubes. (See [5, 7, 23, 24] for recent investigations of partial cubes.) A formula for the Mostar index of arbitrary Cartesian products was then independently given in [2, Theorem 1.5] and in [21, Theorem 3.1]. Our contribution in this section is a short proof of the formula. The short proof reveals how Corollary 2.2 is extremely useful.

Theorem 4.2. If G_1 and G_2 are graphs, then

$$Mo(G_1 \square G_2) = n(G_1)^2 Mo(G_2) + n(G_2)^2 Mo(G_1).$$

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Proof. Set $n_1 = n(G_1)$ and $n_2 = n(G_2)$. Recall the folklore result that the distance function is additive in Cartesian products, that is, $d_G((u_1, u_2), (v_1, v_2)) = d_{G_1}(u_1, v_1) + d_{G_2}(u_2, v_2)$ holds, see [16]. Therefore $\operatorname{Tr}_G((u, v)) = n_2 \operatorname{Tr}_{G_1}(u) + n_1 \operatorname{Tr}_{G_2}(v)$ for any vertex $(u, v) \in V(G)$. Then, by Corollary 2.2,

$$\begin{split} \mathsf{Mo}(G) &= \sum_{u \in V(G_1) \atop vw \in E(G_2)} |\mathrm{Tr}_G((u,v)) - \mathrm{Tr}((u,w))| + \sum_{u \in V(G_2) \atop vw \in E(G_1)} |\mathrm{Tr}_G((v,u)) - \mathrm{Tr}((w,u))| \\ &= \sum_{u \in V(G_1) \atop vw \in E(G_2)} |n_1 \mathrm{Tr}_{G_2}(v) - n_1 \mathrm{Tr}_{G_2}(w)| + \sum_{u \in V(G_2) \atop vw \in E(G_1)} |n_2 \mathrm{Tr}_{G_1}(v) - n_2 \mathrm{Tr}_{G_2}(w)| \\ &= n_1^2 \mathrm{Mo}(G_2) + n_2^2 \mathrm{Mo}(G_1), \end{split}$$

completing the proof of the theorem. \Box

Using simple induction, Theorem 4.2 can be extended to Cartesian products with an arbitrary number of factor graphs. Here we give a formula for the special case of G^k , the Cartesian product of k copies of G.

Corollary 4.3. *If G is a graph with* $n(G) \ge 2$ *, then*

$$Mo(G^k) = kn(G)^{2k-2}Mo(G).$$

4.2. Corona

The *corona product* $G \odot H$ of graphs G and H is the graph obtained by taking one copy of G and n(G) copies of H and joining each vertex of the *i*-th copy of H with the *i*-th vertex of G. In [2, Theorem 1.1] an upper bound on the Mostar index of corona product is given. We next give an exact result.

Theorem 4.4. If G_1 and G_2 are graphs, then

$$Mo(G_1 \odot G_2) = (n(G_2) + 1)Mo(G_1) + n(G_1)^2 n(G_2)(n(G_2) + 1) -n(G_1)(2m(G_2) + n(G_2)) + n(G_1)irr(G_2).$$

Proof. Let $G = G_1 \odot G_2$. For $i \in [2]$ set $V_i = V(G_i)$, $E_i = E(G_i)$, $n_i = n(G_i)$, and $m_i = m(G_i)$. Let further $V(G_1) = \{v_1, \ldots, v_{n_1}\}$, and let $G_{2,i}$ be the copy of G_2 associated with v_i , $i \in [n_1]$. Then

$$\begin{aligned} \mathsf{Mo}(G) &= \sum_{v_i v_j \in E_1} |n_G(v_i) - n_G(v_j)| + \sum_{i=1}^{n_1} \sum_{x \in V(G_{2,i})} |n_G(v_i) - n_G(x)| \\ &+ \sum_{i=1}^{n_1} \sum_{xy \in E(G_{2,i})} |n_G(x) - n_G(y)|. \end{aligned}$$

If $v_i v_j \in E_1$ and if $v_k \in V(G_1)$ is closer to v_i than to v_j in G_1 , then all vertices of $G_{2,k}$ are closer to v_i than to v_j in G. Then it follows that $|n_G(v_i) - n_G(v_j)| = (n_2 + 1)|n_{G_1}(v_i) - n_{G_1}(v_j)|$. If $e = xv_i \in E(G)$, where $x \in V(G_{2,i})$, then all vertices of G, except the vertices adjacent to x, are closer to v_i than to x. Therefore we have $\phi_G(e) = ||V(G)| - \deg_{G_2}(x) - 1| = |n_1(n_2 + 1) - n_1 - \deg_{G_2}(x) - 1|$. Finally consider the edge $f = xy \in E(G_{2,i})$. Since all vertices of $G_{2,i}$ are adjacent to v_i , all the vertices in $V(G) \setminus (N_{G_{2,i}}(x) \cup N_{G_{2,i}}(y))$ have the same distance to x and to y. Thus $\phi(f) = |\deg_{G_2}(x) - \deg_{G_2}(y)|$. Therefore,

$$Mo(G) = \sum_{v_i v_j \in E_1} (n_2 + 1) |n_{G_1}(v_i) - n_{G_1}(v_j)| + \sum_{i=1}^{n_1} \sum_{x \in V(G_{2,i})} [n_1(n_2 + 1) - (\deg_{G_2}(x) + 1)] + \sum_{i=1}^{n_1} \sum_{xy \in E(G_{2,i})} |\deg_{G_2}(x) - \deg_{G_2}(y)| = (n_2 + 1)Mo(G_1) + n_1^2 n_2(n_2 + 1) - n_1(2m_2 + n_2) + n_1 \operatorname{irr}(G_2)$$

completing the proof of the theorem. \Box

The *thorny graph* $G^*(p_1, ..., p_{n(G)})$ of a graph G with parameters $p_1, ..., p_{n(G)}$ is obtained from G by attaching p_i pendant vertices to the *i*-th vertex of G with $i \in [n(G)]$ [15]. (For additional properties of thorny graphs see [22].) If $p_1 = \cdots = p_n = p$, then we simplify the notation to $G^*(p^{(n)})$. Since $G^*(p^{(n)}) \cong G \odot pK_1$, Theorem 4.4 gives:

Corollary 4.5. *If G is a graph, then*

$$Mo(G^*(p^{(n)})) = (p+1)Mo(G) + n(G)^2p(p+1) - n(G)p$$

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