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Steiner (Revised) Szeged Index of Graphs*

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Abstract

The Steiner distance in a graph, introduced by Chartrand et al. in 1989, is a natural generalization of the concept of classical graph distance. For a connected graph G of order at least 2 and $S \subseteq V(G)$, the Steiner distance $d_G(S)$ of the set S of vertices in G is the minimum size of a connected subgraph whose vertex set contains or connects S. In this paper, we introduce the concept of the Steiner (revised) Szeged index $(rSz_k(G))$ $Sz_k(G)$ of a graph G, which is a natural generalization of the well-known (revised) Szeged index of chemical use. We determine the $Sz_k(G)$ for trees in general. Then we give a formula for computing the Steiner Szeged index of a graph in terms of orbits of automorphism group action on the edge set of the graph. Finally, we give sharp upper and lower bounds of $(rSz_k(G))$ $Sz_k(G)$ of a connected graph G, and establish some of its properties. Formulas of $(rSz_k(G))$ $Sz_k(G)$ for large k are also given in this paper.

1 Introduction

All graphs in this paper are assumed to be undirected, finite and simple. We refer to [3] for graph theoretical notation and terminology not specified here. Distance is one of basic concepts in graph theory [4]. If G is a connected graph and $u, v \in V(G)$, then the *distance* $d(u, v) = d_G(u, v)$ between u and v in G is the length of a shortest path of G connecting u and v. For more details on classical distance, see [10].

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Let $e = uv$ be an edge of a graph G. Let $N_u(e|G)$ be the set of vertices of G which are closer to u than to v and let $N_v(e|G)$ be set of those vertices which are closer to v than to u. The set of those vertices which have equal distance from v and u is denoted by $N_0(e|G)$. More formally,

$$N_u(e|G) = \{w \in V(G) : \ d_G(w, u) < d_G(w, v)\},$$

$$N_v(e|G) = \{w \in V(G) : \ d_G(w, v) < d_G(w, u)\}$$

and

$$N_0(e|G) = \{w \in V(G) : \ d_G(w, u) = d_G(w, v)\}.$$

Let $n_u(e) = |N_u(e|G)|$, $n_v(e) = |N_v(e|G)|$ and $n_0(e) = |N_0(e|G)|$. Then the *Szeged index* of a graph G, denoted by $Sz(G)$, is defined as

$$Sz(G) = \sum_{e=uv\in E(G)} n_u(e)n_v(e),$$

and the *revised Szeged index* of a graph G, denoted by $rSz(G)$, is defined as

$$rSz(G) = \sum_{e=uv\in E(G)} (n_u(e) + n_0(e)/2)(n_v(e) + n_0(e)/2).$$

The basic properties of the (revised) Szeged index and bibliography on $(rSz(G))$ $Sz(G)$ are presented in [2, 7, 11, 19, 20].

The Steiner distance of a graph, introduced by Chartrand et al. in [6] in 1989, is a natural and nice generalization of the concept of the classical graph distance. For a graph $G = (V, E)$ and a set $S \subseteq V$ of at least two vertices, *an S-Steiner tree* or *a Steiner tree connecting S* (or simply, *an S-tree*) is a subgraph $T = (V', E')$ of G that is a tree with $S \subseteq V'$. Let G be a connected graph of order at least 2 and let S be a nonempty set of vertices of G. Then the *Steiner distance* $d_G(S)$ in G among the vertices of S (or simply the distance of S) is the minimum size of a connected subgraph whose vertex set contains or connects S. Note that if H is a connected subgraph of G such that $S \subseteq V(H)$ and $|E(H)| = d(S)$, then H is a tree. Clearly, $d_G(S) = \min\{|E(T)|\ , S \subseteq V(T)\}$, where T is a subtree of G. Furthermore, if $S = \{u, v\}$, then $d_G(S) = d(u, v)$ is nothing new, but the classical distance between u and v in G. Clearly, if $|S| = k$, then $d_G(S) \geq k - 1$. For more details on the Steiner distance, we refer to [1, 5, 6, 10, 18].

In [14], Li et al. proposed a generalization of the concept of Wiener index, using Steiner distance. Thus, the *kth Steiner Wiener index* $SW_k(G)$ of a connected graph G is defined by

$$SW_k(G) = \sum_{\substack{S\subseteq V(G)\\ |S|=k}} d(S)\,.$$

For $k = 2$, the Steiner Wiener index coincides with the ordinary Wiener index. It is usual to consider SW_k for $2 \le k \le n-1$, but the above definition implies that $SW_1(G) = 0$ and $SW_n(G) = n-1$ for a connected graph G of order n. For more details on the Steiner Wiener index, we refer to [14–17].

Let G be a connected graph and e an edge of G. For a positive integer k, from the Steiner distance, we define another three sets $N_u(e;k)$, $N_v(e;k)$ and $N_0(e;k)$ as follows.

$$N_u(e;k) = \{S' \subseteq V(G), |S'| = k-1 \,|\, d_G(S' \cup \{u\}) < d_G(S' \cup \{v\}),\ u \notin S',\ v \notin S'\},$$

$$N_v(e;k) = \{S' \subseteq V(G), |S'| = k-1 \,|\, d_G(S' \cup \{v\}) < d_G(S' \cup \{u\}),\ v \notin S',\ u \notin S'\},$$

and

$$N_0(e;k) = \{S' \subseteq V(G), |S'| = k-1 \,|\, d_G(S' \cup \{u\}) = d_G(S' \cup \{v\}),\ u \notin S',\ v \notin S'\}.$$

Let $n_u(e;k) = |N_u(e;k)|$, $n_v(e;k) = |N_v(e;k)|$ and $n_0(e;k) = |N_0(e;k)|$. Then the *kth Steiner Szeged index* of a graph G is defined as

$$Sz_k(G) = \sum_{e=uv\in E(G)} (n_u(e;k)+1)(n_v(e;k)+1).$$

Analogously, the *kth Steiner revised Szeged index* of a graph G is defined as

$$rSz_k(G) = \sum_{e=uv\in E(G)} (n_u(e;k)+n_0(e;k)/2+1)(n_v(e;k)+n_0(e;k)/2+1).$$

Here, one may note that the formula is not the same as the classical Szeged index in form. If $k = 2$, then

$$N_u(e;2) = \{w \in V(G) \,|\, d_G(u,w) < d_G(v,w),\ u \ne w, v \ne w\}.$$

One can see $N_u(e;2) \ne N_u$ since we require $u \ne w$. By our definition, the classical Szeged index $Sz(G)$ can be written as

$$Sz(G) = Sz_2(G) = \sum_{e=uv\in E(G)} (n_u(e;2)+1)(n_v(e;2)+1),$$

where $N_u(e;2) = \{w \in V(G) \,|\, d_G(u,w) < d_G(v,w),\ u \ne w\}$ and $N_v(e;2) = \{w \in V(G) \,|\, d_G(v,w) < d_G(u,w),\ u \ne w\}$.

So, as one can easily see that the Steiner (revised) Szeged index is a natural generalization of the well-known (revised) Szeged index of chemical use.

We proceed as follows. In the next section, we determine the $Sz_k(G)$ for trees in general. Then, we give a formula for computing the Steiner Szeged index of a graph in terms of orbits of automorphism group action on the edge set of the graph. Finally, we give sharp upper and lower bounds of $(rSz_k(G))$ $Sz_k(G)$ of a connected graph G, and establish some of its properties. Formulas of $(rSz_k(G))$ $Sz_k(G)$ for large k are also given.

2 Results for trees

At first, we consider trees. The following result is easy to obtain.

Theorem 2.1. *For a tree T,*

$$Sz_k(T) = \sum_{e=uv\in E(T)} \left(\binom{n_u(e)-1}{k-1}+1\right)\left(\binom{n_v(e)-1}{k-1}+1\right),$$

where $2 \le k \le |V(T)|-1$.

Note that for $k=2$, $Sz_2(T) = \sum_{e=uv\in E(T)} n_u(e)n_v(e) = Sz(T)$, which is exactly the classical Szeged index.

Proof. Let T_u and T_v be the two components of $T-e$. For any $(k-1)$-subset S of $V(T)\setminus\{u,v\}$, if both $S\cap T_u \neq \emptyset$ and $S\cap T_v \neq \emptyset$, then $d_T(S\cup u) = d_T(S\cup v)$. So, $d_T(S\cup u) < d_T(S\cup v)$ if and only if S is in $T_u - u$, and $d_T(S\cup v) < d_T(S\cup u)$ if and only if S is in $T_v - v$. Since $T_u - u$ and $T_v - v$ have $n_u(e)-1$ and $n_v(e)-1$ vertices, respectively, we are thus done. ■

Some examples are given as follows.

Example 2.1. For a path $P_n = u_1u_2\cdots u_iu_{i+1}\cdots u_n$ on vertices, take an edge $e = u_iu_{i+1}$. Then $P_n - e$ has two subpaths P_i and P_{n-i}. So we have $n_{u_i}(e) = i$ and $n_{u_{i+1}}(e) = n-i$. Therefore,

$$Sz_k(P_n) = \sum_{i=1}^{n-1}\left(\binom{i-1}{k-1}+1\right)\left(\binom{n-i-1}{k-1}+1\right).$$

Since any $(k-1)$-subset S of $V(T)\setminus\{u,v\}$ satisfies $d_T(S\cup u) = d_T(S\cup v)$ if and only if both $S\cap T_u \neq \emptyset$ and $S\cap T_v\neq\emptyset$, then we can deduce that

$$n_0(e;k) = \sum_{j=1}^{k-2}\binom{i-1}{j}\binom{n-i-1}{k-j-1}.$$

From this one can give an explicit formula for the $rSz_k(P_n)$. ■

Example 2.2. For the star graph S_{n+1} on $n+1$ vertices with a central vertex u and the other pendant vertices $u_1, u_2, \cdots, u_n$, take an edge $e = uu_i$. Then $S_{n+1} - e$ has two subgraphs $T_{u_i} = P_1$ and $T_u = S_n$. So we have $n_{u_i}(e) = 1$ and $n_u(e) = n$. Therefore,

$$Sz_k(S_{n+1}) = \sum_{i=1}^{n}\left(\binom{n-1}{k-1}+1\right) = n\binom{n-1}{k-1}+n.$$

Since any $(k-1)$-subset S of $V(S_{n+1})\setminus\{u,u_i\}$ satisfies $d_T(S\cup u) = d_T(S\cup u_i)$ if and only if both $S\cap T_u\neq\emptyset$ and $S\cap T_{u_i}\neq\emptyset$, then we have $n_0(e;k)=0$ for any $e = uu_i$ because $T_{u_i} - u_i = \emptyset$, and hence there is no such an S. Therefore, we have

$$rSz_k(S_{n+1}) = Sz_k(S_{n+1}) = n\binom{n-1}{k-1}+n.$$

This will be re-obtained next section by using symmetry on graphs. ■

Remark 2.1. For $k = 2$, the Steiner Szeged index Sz_2 of a tree is equal to the Szeged index Sz, and the Steiner Wiener index SW_2 is equal to the Wiener index W, and hence the Steiner Szeged index Sz_2 of a tree is equal to the Steiner Wiener index SW_2 of a tree since $Sz = W$ for a tree. However, for $k \geq 3$, one can see from Examples 2.1 and 2.2 that the Steiner Szeged index Sz_k of a tree is not equal to the Steiner Wiener index SW_k of a tree.

Conjecture 2.1. For any two trees T and T', $Sz_k(T) \leq Sz_k(T')$ if and only if $Sz(T) \leq Sz(T')$?

3 Results for graphs with symmetry

Let G be a group and Ω be a non-empty set. An action of G on Ω, denoted by $(G|\Omega)$, induces a group homomorphism φ from G into the symmetric group S_Ω on Ω, where $\varphi(g)^\alpha = g^\alpha$, $(\alpha \in \Omega)$. The *orbit* of an element $\alpha \in \Omega$ is denoted by α^G and it is defined as the set of all $\alpha^g, g \in G$.

A bijection σ on the vertex set of a graph Γ is named an *graph automorphism* if it preserves the edge set of Γ. In other words, σ is a graph automorphism of Γ if $e = uv$ is an edge of Γ if and only if $\sigma(e) = \sigma(u)\sigma(v)$ is an edge of Γ. Let $Aut(\Gamma)$ be the set of all graph automorphisms of Γ. Then $Aut(\Gamma)$ under the composition of mappings forms a group. A graph Γ is called *vertex-transitive* if $Aut(\Gamma)$ acting on $V(G)$ has one orbit. We can similarly define an edge-transitive graph just by considering $Aut(\Gamma)$ acting on $E(G)$.

By a minimal tree for a sequence of vertices $(v_1, \cdots, v_n)$, we mean a tree containing the vertices $(v_1, \cdots, v_n)$ which has the minimum number of edges.

Theorem 3.1. *Let $E_1, \cdots, E_r$ be the orbits of a graph Γ under the action of $Aut(\Gamma)$ on the edge set $E(\Gamma)$ of Γ. Suppose $e = uv$ and $f = xy$ are two arbitrary edges of E_i $(1 \leq i \leq r)$. Then $\{n_u(e;k), n_v(e;k)\} = \{n_x(f;k), n_y(f;k)\}$.*

Proof. Since e and f are in the same obit, there is an automorphism $\varphi \in Aut(\Gamma)$ such that $\varphi(u) = x$ and $\varphi(v) = y$. For every minimal tree T containing the vertices $(u, u_1, \cdots, u_{k-1})$, $\varphi(T)$ is a minimal tree that contains $(x, \varphi(u_1), \cdots, \varphi(u_{k-1}))$. This means that if $\{u_1, \cdots, u_{k-1}\} \in N_u(e;k)$, then $\{\varphi(u_1), \cdots, \varphi(u_{k-1})\} \in N_{\varphi(u)}(f;k)$. Thus $n_u(e;k) = |N_u(e;k)| = |N_{\varphi(u)}(f;k)| = n_x(e;k)$. By a similar argument, one can see that $n_v(e;k) = |N_v(e;k)| = |N_{\varphi(v)}(f;k)| = n_y(e;k)$. This means that $\{n_u(e;k), n_v(e;k)\} = \{n_x(f;k), n_y(f;k)\}$. ■

The following corollary is immediate.

Corollary 3.2. *Let $E_1, \cdots, E_r$ be the orbits of a graph Γ under the action of $Aut(\Gamma)$ on the edge set $E(\Gamma)$ of Γ and $u_iv_i = e_i \in E_i$. Then*

$$Sz_k(\Gamma) = \sum_{i=1}^{r} |E_i|(n_{u_i}(e_i;k)+1)(n_{v_i}(e_i;k)+1),$$

and

$$rSz_k(\Gamma) = \sum_{i=1}^{r} |E_i|(n_{u_i}(e_i;k)+n_0(e_i;k)/2+1)(n_{v_i}(e_i;k)+n_0(e_i;k)/2+1).$$

Example 3.1. Suppose K_n is the complete graph on n vertices. It is not difficult to see that for any $uv = e \in E(K_n)$, we have $n_u(e;k) = n_v(e;k) = 0$ and $n_0(e;k) = \binom{n-2}{k-1}$. Then

$$Sz_k(K_n) = \sum_{e=uv\in E(K_n)} (n_u(e;k)+1)(n_v(e:k)+1) = |E(K_n)| = n(n-1)/2,$$

and

$$\begin{aligned} rSz_k(K_n) &= \sum_{e=uv\in E(K_n)} (n_u(e;k)+n_0(e;k)/2+1)(n_v(e;k)+n_0(e;k)/2+1) \\ &= |E(K_n)|\binom{n-2}{k-1}^2. \end{aligned}$$

■

Example 3.2. Suppose $K_{1,n}$ is the star graph on $n+1$ vertices. Let $V(K_{1,n}) = \{u, u_1, \cdots, u_n\}$ and $E(K_{1,n}) = \{\{u,u_1\}, \cdots, \{u,u_n\}\}$. Again $K_{1,n}$ is edge-transitive and for any edge $uu_i = e_i \in E(K_{1,n})$, we have $n_u(e;k) = \binom{n-1}{k-1}$, $n_{u_i}(e;k) = 0$ and $n_0(e;k) = 0$. Then

$$rSz_k(K_{1,n}) = Sz_k(K_{1,n}) = \sum_{e\in E(K_n)} \left(\binom{n-1}{k-1}+1\right) = n\binom{n-1}{k-1}+n.$$

See **Example 2.2**, we get the same result. ■

For complete multipartite graphs, we can get the exact value for the kth Steiner Szeged index.

Theorem 3.3. *Let $\Gamma = K_{a_1,a_2,\ldots,a_m}$ be a complete multipartite graph and let k be an integer such that $k \le a_i$ $(1 \le i \le m)$. Then*

$$Sz_k(\Gamma) = \sum_{i=1}^{m-1}\sum_{j=i+1}^{m} a_ia_j \left(\binom{a_i-1}{k-1}+1\right)\left(\binom{a_j-1}{k-1}+1\right),$$

and

$$rSz_k(\Gamma) = \sum_{i=1}^{m-1}\sum_{j=i+1}^{m} a_ia_j\left(\binom{a_i-1}{k-1} + n_0(e;k)/2+1\right)\left(\binom{a_j-1}{k-1} + n_0(e;k)/2+1\right),$$

where $B = V(\Gamma) - (A_i \cup A_j)$ *and*

$$n_0(e;k) = \binom{|B|}{k-1} + \sum_{p=1}^{a_i-2}\sum_{q=1}^{k-1-p}\binom{a_i-2}{p}\binom{a_j-1}{q}\binom{|B|}{k-1-(p+q)}.$$

Proof. For $\Gamma = K_{a_1,a_2,\dots,a_m}$, let A_t $(1 \le t \le m)$ be the multi-partition of Γ such that $A_t = \{a_{t1}, a_{t2}, \dots, a_{ta_t}\}$. Consider two different parts A_i and A_j, where $1 \le i,j \le m$ and $a_i \le a_j$. First, let $k \le a_i$ and consider the edge $e = uv$ such that $u \in A_i$ and $v \in A_j$. Suppose that $W \subseteq V(\Gamma)$, where $|W| = k-1$. Let $W \subseteq A_i$ such that $u \notin W$ and without loss of generality, we can suppose $W = \{a_{i1}, a_{i2}, \dots, a_{i(k-1)}\}$. Then the tree induced by the edges $\{va_{i1}, va_{i2}, \dots, va_{i(k-1)}, vu\}$ is the Steiner tree containing u and the tree induced by the edges $\{va_{i1}, va_{i2}, \dots, va_{i(k-1)}\}$ is the Steiner tree containing v. So, $d_S(v) < d_S(u)$. Similarly, if $W \subseteq A_j$, then $d_S(u) < d_S(v)$. Let $W = \{w_1, w_2, \dots, w_{k-1}\} \subseteq V(\Gamma)$ such that $W \cap (A_i \cup A_j) = \phi$. So, the tree induced by the edges $\{uw_1, uw_2, \dots, uw_{(k-1)}\}$ is the Steiner tree containing u and the tree induced by the edges $\{vw_1, vw_2, \dots, vw_{(k-1)}\}$ is the Steiner tree containing v. This means that $d_S(v) = d_S(u)$. Also, if $|W \cap A_i| = p$, $|W \cap A_j| = q$ and $|W \cap (V(\Gamma) - (A_i \cup A_j))\,| = l$, where $W = \{a_{i1}, a_{i2}, \dots, a_{ip}, a_{j1}, a_{j2}, \dots, a_{jq}, w_1, w_2, \dots, w_l\}$ $(p+q+l = k-1)$, then $\{ua_{j1}, \dots, ua_{jq}, uw_1, \dots, uw_l, w_1a_{i1}, \dots, w_1a_{ip}\}$ is the Steiner trees containing u and $\{va_{i1}, \dots, va_{ip}, vw_1, \dots, vw_l, w_1a_{j1}, \dots, w_1a_{jq}\}$ is the Steiner trees containing v. This implies that $d_S(v) = d_S(u)$. By the above discussion we have that $n_v(e;k) = \binom{a_i-1}{k-1}$ and $n_u(e;k) = \binom{a_j-1}{k-1}$. So,

$$Sz_k(\Gamma) = \sum_{i=1}^{m-1}\sum_{j=i+1}^{m} a_ia_j\left(\binom{a_i-1}{k-1}+1\right)\left(\binom{a_j-1}{k-1}+1\right).$$

Assume that $B = V(\Gamma) - (A_i \cup A_j)$. Then $n_0(e;k) = X + Y$, where

$$X = \binom{|B|}{k-1} \text{ and } Y = \sum_{p=1}^{a_i-2}\sum_{q=1}^{k-1-p}\binom{a_i-2}{p}\binom{a_j-1}{q}\binom{|B|}{k-1-(p+q)}.$$

This completes the proof. ■

4 Formulas for large *k*

For trees, we have the following formula for $k = n - 1$.

Theorem 4.1. *Let T be a tree of order n with p pendent edges. Then*

$$Sz_{n-1}(T) = n + p - 1$$

and

$$rSz_{n-1}(T) = 2p + \frac{9}{4}(n - p - 1).$$

Proof. Let $e = uv$ be an edge of T. If e is not a leaf, then $|N_u(e; n-1)| = |N_v(e; n-1)| = 0$. Suppose e is a leaf and u is a pendent vertex. Then v is a cut vertex. Then $|N_v(e; n-1)| = 1$ and $|N_u(e; n-1)| = 0$, and hence

$$Sz_{n-1}(T) = (n - 1 - p) + 2p = n + p - 1$$

and

$$rSz_{n-1}(T) = 2p + \frac{9}{4}(n - p - 1).$$

■

Remark 4.1. Notice that the derivative function $(rSz_{n-1})'(T)$ is less than zero thus the function $rSz_{n-1}(T) = 2p + \frac{9}{4}(n - p - 1)$ is strictly increasing. Let $\mathcal{T}_n$ be all of trees with n vertices. Among all elements of $\mathcal{T}_n$, the star graph S_n and the path graph P_n has the minimum and the maximum value of rSz_{n-1}, respectively. ■

The following observation is immediate for $k = n - 1$.

Theorem 4.2. *Let G be a connected graph of order n and size m with p pendent edges. Then*

$$Sz_{n-1}(G) = p + m.$$

and

$$rSz_{n-1}(G) = 2p + \frac{9}{4}(m - p).$$

Proof. Let $e = uv$ be an edge of T. If e is not a pendent edge, then $|N_u(e; n-1)| = |N_v(e; n-1)| = 0$. Suppose e is a pendent edge and u is a pendent vertex. Then v is a cut vertex. Then $|N_v(e; n-1)| = 1$ and $|N_u(e; n-1)| = 0$, and hence

$$Sz_{n-1}(T) = (m - p) + 2p = p + m.$$

and

$$rSz_{n-1}(G) = 2p + \frac{9}{4}(m - p).$$

■

5 Upper and lower bounds

For general graphs, we have the following upper and lower bounds.

Theorem 5.1. *Let n, k be two integers with $2 \leq k \leq n-1$, and let G be a graph of order n and size m.*

(1) If G is $(n-k)$-connected, then

$$Sz_k(G) = m.$$

(2) If G is not $(n-k)$-connected, then

$$m \leq Sz_k(G) \leq m\left(\left\lceil \frac{1}{2}\binom{n-2}{k-1}\right\rceil + 1\right)\left(\left\lfloor \frac{1}{2}\binom{n-2}{k-1}\right\rfloor + 1\right).$$

Proof. (1) Let uv be an edge of G. Since G is $(n-k)$-connected, it follows that for any $S \subseteq V(G)$ and $|S'| = k-1$, $d_G(S \cup \{u\}) = d_G(S \cup \{v\}) = k$, and hence $|N_u(e;k)| = |N_v(e;k)| = 0$. So $Sz_k(G) = m$.

(2) From the definition, we have

$$Sz_k(G) = \sum_{uv \in E(G)} (n_u(e;k)+1)(n_v(e;k)+1) \geq \sum_{e=uv \in E(G)} 1 = e(G) = m.$$

and

$$\begin{aligned} Sz_k(G) &= \sum_{uv \in E(G)} (n_u(e;k)+1)(n_v(e;k)+1) \\ &\leq \sum_{uv \in E(G)} \left(\left\lceil \frac{1}{2}\binom{n-2}{k-1}\right\rceil + 1\right)\left(\left\lfloor \frac{1}{2}\binom{n-2}{k-1}\right\rfloor + 1\right) \\ &= m\left(\left\lceil \frac{1}{2}\binom{n-2}{k-1}\right\rceil + 1\right)\left(\left\lfloor \frac{1}{2}\binom{n-2}{k-1}\right\rfloor + 1\right). \end{aligned}$$

■

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