Research Article

Certain Distance-Based Topological Indices of Parikh Word Representable Graphs

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Relating graph structures with words which are finite sequences of symbols, Parikh word representable graphs (PWRGs) were introduced. On the other hand, in chemical graph theory, graphs have been associated with molecular structures. Also, several topological indices have been defined in terms of graph parameters and studied for different classes of graphs. In this study, we derive expressions for computing certain topological indices of PWRGs of binary core words, thereby enriching the study of PWRGs.

1. Introduction

Among various studies that involve graphs for analyzing and solving different kinds of problems, relating words that are finite sequences of symbols with graphs is an interesting area of investigation (for example, [1–5]). Based on the notion of subwords (also called scattered subwords) of a word and the concept of a matrix called Parikh matrix of a word, introduced in [6] and intensively investigated by many researchers (for example, [7–13] and references therein) with entries of the Parikh matrix giving the counts of certain subwords in a word, a graph called Parikh word representable graph (PWRG) of a word, was introduced in [14] and its relationship with the corresponding word and partition was studied in [15].

On the other hand, there has been a great interest in various topological indices associated with graphs (for example, [16–19]) due to their application in the area of chemical graph theory [20], which deals with representations of organic compounds or equivalently their molecular structures as graphs, with atoms other than hydrogen often represented by vertices and covalent chemical bonds by edges. In fact, in chemical graph theory, there have been attempts to capture the molecular structure in terms of the topological index of the corresponding graph.

There are a number of studies (for example, [21]) of various topological indices of graphs establishing formulae for computing the indices and also providing upper and lower bounds on the values of such indices. Recently, in [22], properties of one of the important topological indices, namely, Wiener index and some of its variants related to PWRGs of binary words, were studied. In this study, certain distance-based topological indices of PWRGs of binary core words are investigated.

2. Preliminaries

The basic definitions and notations relating to words are as given in [23, 24]. We recall here some of the needed notions.

An ordered alphabet $\Sigma$ is a set of symbols with an ordering on its symbols. For example, $\Sigma = \{a_1, a_2, \ldots, a_k\}$ with an ordering $a_1 < a_2 < \cdots < a_k$ is an ordered alphabet, written
as \( \Sigma = \{a_1 < a_2 < \cdots < a_k\} \). A word \( w \) over \( \Sigma \) is a finite sequence of symbols belonging to \( \Sigma \). A word \( w' \) is a scattered subword or simply called a subword of a word \( w \) over \( \Sigma \) if and only if there exist \( u_1, u_2, \ldots, u_m, u_i \in \Sigma \) for \( 1 \leq i \leq n \) and words (possibly empty) \( v_0, v_1, \ldots, v_m \) over \( \Sigma \), such that \( w = u_1 v_1 u_2 v_2 \cdots u_m v_m \). The number of occurrences of a word \( u \) as a subword of \( w \) is denoted by \( |w|_u \). For example, in the word \( w = aababab \) over the ordered binary alphabet \{a < b\}, the number of \( a's \) is \( |w|_a = 3 \), the number of \( b's \) is \( |w|_b = 3 \), and the number of subwords \( ab \)'s is \( |w|_{ab} = 8 \). In fact, the word \( ab \) as a subword of aababb is shown with the symbols \( a \) and \( b \) of \( ab \) shown in bold in aababb.

\[
aababb, aababb, aababb, aababb, aababb, aababb, aababb, aababb, aababb. 
\]  

(1)

The set of all words over an alphabet \( \Sigma \), including the empty word \( \lambda \) with no symbols, is denoted by \( \Sigma^* \). Unless stated otherwise, we consider only a binary alphabet \( \Sigma = \{a < b\} \).

**Definition 1.** [13] Let \( w \in \Sigma^* \). The core of \( w \), denoted by \( \text{core}(w) \), is the unique word \( w_0 \) of \( w \) with the smallest possible length, such that \( \text{core}(w) \in w^* \). A word \( w \in \Sigma^* \) is called a core word if and only if \( \text{core}(w) = w \).

Clearly, a nonempty binary word \( w \in \Sigma^* \) is a core word if and only if \( w \) starts with \( a \) and ends with \( b \).

In [14], a simple graph, called Parikh word representable graph (PWRG), was defined corresponding to a word over an ordered alphabet. Restricting our attention to binary words, we recall now this PWRG.

**Definition 2.** [14] For a binary word \( w \) of length \( n \) over \( \Sigma = \{a < b\} \), we define a simple graph \( G = G(w) \), called Parikh word representable graph (PWRG), with \( n \) labeled vertices \( 1, 2, \ldots, n \) representing the positions of the consecutive letters of \( w \), such that for each occurrence of the subword \( ab \) in \( w \), there is an edge between the vertices in \( G \), corresponding to the positions of \( a \) and \( b \) in \( w \). We say that the binary word \( w \) represents the graph \( G = G(w) \) and a graph \( G \) is Parikh word representable if there exists a binary word \( w \) that represents \( G \).

It is to be noted that PWRG \( G(w) \) of a binary word \( w \) over \{a < b\} is a bipartite graph [14] with as many vertices as the length \( |w| \) of \( w \) and as many edges as the number of occurrences of the subword \( ab \) in \( w \). Figure 1 shows the PWRG of a binary word aababab over the ordered binary alphabet \( \Sigma = \{a < b\} \). The graph \( G(aababab) \) has 7 vertices and 9 edges. Note that the length of the word aababab has 7 vertices and there are 9 occurrences of the subword ab in aababab.

In this study, we deal with only binary core words and the corresponding PWRGs. Also, we note that for a nonempty binary core word of the form \( w = a_{n_1}^1 b a_{n_2}^1 b \cdots a_{n_k}^1 b \), where \( n_1 \geq 1 \) and \( n_k \) is nonnegative for each \( k, 2 \leq k \leq |w|_b \), the number of edges in the corresponding PWRG \( G(w) \) is

\[
|w|_{ab} = (n_1 + n_2 + \cdots + n_{|w|_b}) + \cdots + (n_1 + n_2) + n_1. 
\]  

(2)

Note that in the word \( w_i, n_k, 1 \leq k \leq |w|_l, \) which is a power of \( a \), indicates that there are \( n_k \) vertices labeled \( a \) in the graph \( G(w) \) with each of these joined to all the vertices that correspond to the subsequent \( b's \) in the word \( w \).

### 3. Distance-Based Topological Indices

We consider only simple graphs, and for notions related to graphs, we refer to [25]. Let \( G = (V, E) \) be a connected graph with vertex set \( V(G) = V \) and edge set \( E(G) = E \). The distance between the vertices \( u \) and \( v \) of \( G \), denoted by \( d(u, v) \), is defined as the length of a shortest path between \( u \) and \( v \) in \( G \). The degree of a vertex \( u \) of \( G \), which is the number of edges adjacent to \( u \), is denoted by \( \deg(u) \). For a given vertex \( u \) in a connected graph \( G \), the eccentricity \( e(u) \) is defined as the maximum distance between \( u \) and any other vertex in \( G \).

**Definition 3.** [26] The Harary index of a connected graph \( G \) is defined as the sum of the reciprocals of distances between all pairs of vertices of \( G \), i.e.,

\[
H(G) = \sum_{|u,v| \in V(G)} \frac{1}{d(u,v)} 
\]  

(3)

The Harary index [26] of a connected graph is a topological index which has been extensively investigated (for example, [27–29]).

**Theorem 1.** The Harary index of the PWRG \( G(w) \), for \( w = a^n b a^n b \cdots a^n b, n_1 \geq 1, n_k \geq 0 \) for \( 2 \leq k \leq |w|_l \), is given by

\[
H(G(w)) = \frac{1}{12} (|w|_a (|w|_a - 1) + 3|w|_b (|w|_b - 1) + 8|w|_{ab} + 4|w|_b |w|_b).
\]  

(4)

**Proof.** We consider pairs of vertices \( (u, v) \) in the PWRG \( G(w) \) corresponding to the word \( w = a^n b a^n b \cdots a^n b \), with \( u, v \in \{1, 2, \ldots, n_l\} \), where the label of \( u \) appears before the label of \( v \) in \( w \). There are now four cases to be considered. We will refer to a pair \( (u, v) \) of such vertices with

(i) Both \( u \) and \( v \) labeled \( a 
(ii) \( u \) labeled \( a \) and \( v \) labeled \( b 
(iii) \( u \) labeled \( b \) and \( v \) labeled \( a 
(iv) Both \( u \) and \( v \) labeled \( b 

Figure 1: The PWRG of the word aababab.
They are given as a pair of type 1, 2, 3, and 4, respectively. There are \((n_1 + n_2 + \cdots + n_l)C_2 = |w_a|C_2 = (1/2)|w_a|\)
\((|w_a| - 1)\) pairs of vertices of type 1 and \(|w_a|C_2 = (1/2)|w_b|(|w_b| - 1)\) of type 4, and the distance between each such pair is 2. Here, \(nC_2\) is the binomial representing the number of ways of choosing \(r\) objects from \(n\) objects. There are \(l_1 + (l - 1)n_2 + \cdots + n_l = |w|_{ab}\) pairs of vertices of type 2 with distance 1 and \(n_1 + 2n_3 + \cdots + (l - 1)n_l = |w_a|w_b - |w|_{ab}\) pairs of vertices of type 3 with distance 3, since \(|w|_{ab} = (n_1 + n_2 + \cdots + n|w_{ab}|) + \cdots + (n_1 + n_2) + n_1.\)

Therefore, \(H(G(w)) = \frac{1}{4}(|w_a|(|w_a| - 1) + |w_b|(|w_b| - 1))\)
\(\quad + |w|_{ab} + \frac{1}{3}(|w_a||w_b| - |w|_{ab})).\)

which yields the required result.

**Theorem 2.** The Harary index \(H(G(w))\) of a PWRG \(G(w) = (V_1 \cup V_2, E)\) with \(|V_1| = |w_a| = p, |V_2| = |w_b| = q\) for the word \(w = a^n b a^n b, \ldots, a^n b, n_1 \geq 1, n_k \geq 0\)
for \(2 \leq k \leq l\), is bounded by
\(\frac{1}{12}(3p^2 + 3q^2 + 4pq + 5p + 5q - 8),\) 
and above by
\(\frac{1}{4}(p^2 + q^2 + 4pq - p - q).\)

where \(k\) be the number of \(b\)'s succeeding the last \(a\) in \(w\).

**Proof.** Let \(G(w)\) be the PWRG corresponding to \(w = a^n b a^n b, \ldots, a^n b\). Then, the vertices representing all \(a\)'s preceding the first \(b\) and all \(b\)'s succeeding the last \(a\) are of eccentricity two, whereas the eccentricity of each of the remaining vertices is three. The vertices \(u\) and \(v\) in \(G(w)\) are adjacent if and only if \(u\) represents \(a\) and \(v\) represents \(b\), such that the position of \(b\) in \(w\) is greater than the position of \(a\) in \(w\). This implies that the contribution to the eccentric connectivity index from the vertices in \(G(w)\) represents

(i) \(a\)'s in the first block \(a^n b\) is \(2n_1|w_a|\), as each vertex corresponding to \(a\) has degree \(|w_a|\)
(ii) \(b\)'s succeeding the last \(a\) is \(2k|w_a|\) (where \(k \geq 1\) is the number of \(b\)'s succeeding the last \(a\)) as each vertex corresponding to such \(ab\) has degree \(|w_a|\) and

The bounds are attained on \(G(ab^{l-1}a^{p-1}b)\) and \(G(a^p b^{l-1})\), respectively.

**Proof.** Since \(G(w)\) is connected, \(|w|_{ab} = |E| \geq p + q - 1\) [25]. Also, \(|w|_{ab} \leq pq\) [6]. Hence, from Theorem 1, the Harary index of \(G(w)\) is
\[H(G(w)) \leq \frac{1}{12}(3p^2 + 3q^2 + 12pq - 3p - 3q)\]
\[= \frac{1}{4}(p^2 + q^2 + 4pq - p - q),\]
which is the Harary index of the PWRG \(G(ab^{l-1}b)\) and
\[H(G(w)) \geq \frac{1}{12}(3p^2 + 3q^2 + 4pq + 5p + 5q - 8),\]
which is the Harary index of the PWRG \(G(a^{p-1}a^{l-1}b)\).

**Definition 4.** [30] The eccentric connectivity index of a connected graph \(G\) with vertex set \(V\) is defined as \(\zeta_c(G) = \sum_{v \in V} e(v)\deg(v)\), where \(e(v)\) is the eccentricity of \(v\).
The total eccentricity index [31] of the graph \(G\) is \(\zeta(G) = \sum_{v \in V} e(v)\).
The topological index, namely, eccentric connectivity index, was introduced in [30] and has been widely investigated for different classes of graphs (for example, [32–35] and references therein).

**Theorem 3.** The eccentric connectivity index of the PWRG \(G(w)\), for \(w = a^n b a^n b, \ldots, a^n b, n_1 \geq 1\), is given by

\[\zeta_c(G(w)) = \begin{cases} 6|w_a| - k|w_a| - n_1|w_b|, & \text{if } |w|_a > 1 \text{ and } |w|_b = l > 1, \\ 3|w_b|, & \text{if } n_1 = 1, n_i = 0, \text{ for } 1 < i \leq l \text{ and } l > 1, \\ 3|w_a|, & \text{if } n_1 > 1 \text{ and } l = 1, \\ 2, & \text{if } n_1 = 1, l = 1, \\ \end{cases}\]

(iii) The remaining \(a\)'s and \(b\)'s in \(w\) is
\[3(2|w|_{ab} - n_1|w|_b - k|w|_a),\] since the sum of the degrees of all vertices in \(G(w)\) is \(2|w|_{ab}\)

Therefore,
\[\zeta_c(G(w)) = 2n_1|w|_b + 2k|w|_a + 3(2|w|_{ab} - n_1|w|_b - k|w|_a)\]
\[= 6|w|_{ab} - n_1|w|_b - k|w|_a.\]

Now, if \(n_1 = 1\) and \(n_i = 0\) for \(1 < i \leq l\), then \(w = ab^l\), and \(a\) is of eccentricity one and degree \(l\) and each \(b\) is of eccentricity two and degree one.

Then,
\[\zeta_c(G(w)) = 3|w|_b, \text{ if } n_1 = 1 \text{ and } n_i = 0, 1 < i \leq l.\]

Similarly, if \(n_1 > 1\) and \(l = 1\), \(w = a^n b\) and \(b\) is of eccentricity one and degree \(n_1\), while each \(a\) is of eccentricity two and degree one. Thus, \(\zeta_c(G(w)) = 3|w|_a.\) Again, if \(n_1 = 1\)
and $l = 1$, then $w = ab$, and both vertices have eccentricity one and degree one and so $\zeta_c(G(w)) = 2$. Hence the result. □

**Remark 1.** It can be seen that the total eccentricity index of the PWRG corresponding to eccentricity 3 and degrees $\eta's$ and $\delta's$ as possible to the left and as many $b's$ as possible to the right of the word, thus providing maximum eccentricity for the vertices in the PWRG corresponding to the $a's$ and $b's$ in $a^p b^q$ which have eccentricity 3. In fact, more formally, for $w = a^n b a^{n-1} b \ldots a b^n b$, $n_1 \geq 1, \eta > 0$, and below by $\zeta_c^{\min}$ where

$\zeta_c^{\max} = \begin{cases} 
4pq, & \text{if } p + q \leq 6, \\
4pq + p + q - 6, & \text{if } p + q \geq 6 \text{ and } 2pq - 8p - 8q + 24 \leq 0, \\
6pq - 7p - 7q + 18, & \text{if } p + q > 6 \text{ and } 2pq - 8p - 8q + 24 \geq 0,
\end{cases}$

$\zeta_c^{\min} = 5p + 5q - 6.$

The upper bound is attained on $G(a^p b^q)$ when $p + q \leq 6$, on $G(a^p b^{p-1} b^{q-1})$ when $p + q > 6, 2pq - 8p - 8q + 24 \leq 0$, and on $G(ab a^{p-2} b^{q-2} b)$ when $p + q > 6, 2pq - 8p - 8q + 24 \geq 0$, while the lower bound is attained on $G(ab a^{p-1} a b^{q-1} b)$.

**Theorem 4.** The eccentric connectivity index $\zeta_c(G(w))$ of a PWRG $G(w) = (V_1 \cup V_2, E)$ with $|V_1| = |w|_a = p, |V_2| = |w|_b = q > 1$ for the word $w = a^n b a^n b \ldots a^p b^n b$, $n_1 \geq 1, \eta_0 \geq 0$ for $2 \leq i \leq q$, is bounded above by $\zeta_c^{\max}$ and below by $\zeta_c^{\min}$ where

In order to maximize this expression with the constraint $n_1 + n_2 + \cdots + n_{q-1} + n_q = p > 1$, we have to minimize the negative terms, and so we have to take $n_1 = n_q = 1$ and $n_2 = p - 2$, while $n_i = 0$, for $3 \leq i \leq q - 1$. Note that we cannot choose $n_2 = 0$ as there are $p > 1$ number of $a's$. Hence, it may be observed that for given values of $p$ and $q$, the maximum value of $\zeta_c(G(w))$ is attained on one of the three words $w_1 = a^p b^q, w_2 = a^{p-1} b b^{q-1}$, or $w_3 = a b a^{p-2} b^{q-2} b$ whose corresponding PWRGs $G(w_1), G(w_2), G(w_3)$ have their eccentric connectivity indices as $n_1 = 4pq, n_2 = 4pq + p + q, n_3 = 6pq - 7p - 7q + 18, \ldots, n_{q-1} = (q - 1)n_q$. Hence, the maximum value is attained on $G(ab a^p b^q)$ when $p + q \leq 6$, on $G(ab a^{p-1} b b^{q-1})$ when $p + q > 6, 2pq - 8p - 8q + 24 \leq 0$, on $G(ab a^{p-2} b b^{q-2} b)$ when $p + q > 6$ and $2pq - 8p - 8q + 24 > 0$.

On the other hand, for $p + q > 1$, $\zeta_c(G(w))$ is minimum when $|w|_{ab}$ is minimum, and this happens for $w = a^n b a^{n-1} b \ldots a b^{n-1} b$ with $|w|_{ab} = n_1 q + pk - n_1 k$ minimum when $n_1 = k = 1$. Hence, the minimum value $5p + 5q - 6$ of $\zeta_c(G(w))$ is attained on $G(ab a^{p-1} a b^{q-1} b)$.

**Theorem 5.** The total eccentricity index $\zeta(G(w))$ of a PWRG $G(w) = (V_1 \cup V_2, E)$ with $|V_1| = |w|_a = p, |V_2| = |w|_b = q$ for the word $w = a^n b a^n b \ldots a^{n_a} b^n b$, $n_1 \geq 1, n_0 \geq 0$ for $2 \leq i \leq q$, is bounded above by $3p + 3q - 2$ and below by
2p + 2q. This upper bound is attained on G(w), for any word w = abuab, where |w|_a = p − 2, |w|_b = q−2. In particular, it is achieved on G(ab^r1a_p−1b). The lower bound is achieved on G(a^p b^q).

Proof. If k is the number of b's following the last a in w, it is clear that the maximum value of \( \xi_G(w) \) is attained when \( n_1 = 1, k = 1 \) and the minimum is attained when \( n_1 = p, k = a \). Hence the result.

Yet another topological index, called eccentric connectivity connectivity coindex \([36, 37]\) of a connected graph, is defined as the eccentricity sum of all nonadjacent vertex pairs in the graph. We consider this index here for PWRGs. 

\[
\xi_c(G(w)) = \begin{cases} 
(l|w| - 1)(3|w| - n_1 - k) - 6|w|_{ab} + k|w|_a + n_1|w|_b, & \text{if } |w|_a > 1, l > 1 \\
2|w|_b(|w|_b - 1), & \text{if } n_1 = 1, n_1 = 0, 0 < i < l, l > 1 \\
2|w|_a(|w|_a - 1), & \text{if } n_1 > 1, l = 1 \\
0, & \text{if } n_1 = 1, l = 1,
\end{cases}
\]

where \( k \) is the number of b's succeeding the last a in w.

Proof. It has been shown \([36, 37]\) that \( \xi_c(G) = \sum_{u \in V(G)} \epsilon(u)(n_1 - \deg(u)) \) which can be written as \( \xi_c(G) = (n_1 - 1)\sum_{u \in V(G)} \epsilon(u) - \xi_c(G) \), where \( n \) is the number of vertices in the graph G and \( \epsilon(u) \) is the eccentricity of the vertex u. If \( |w|_a > 1 \) and \( l > 1 \), then the vertices corresponding to the first block a's and k b's succeeding the last a are of eccentricity two, and the remaining vertices are of eccentricity three.

Therefore,

\[
\xi_c(G(w)) = (|w| - 1)(3|w| - n_1 - k) - 6|w|_{ab} + k|w|_a + n_1|w|_b.
\]

(18)

Now, if \( n_1 = 1, n_1 = 0 \) for \( 1 < i < l \) and \( l > 1 \), then the vertex corresponding to a is of eccentricity one and the remaining vertices are of eccentricity two.

Therefore, \( \xi_c(G(w)) = 2|w|_b(|w|_b - 1) \).

Now, if \( n_1 > 1 \) and \( l = 1 \), then the vertex corresponding to b is of eccentricity one and the remaining vertices are of eccentricity two. Then, \( \xi_c(G(w)) = 2|w|_a(|w|_a - 1) \).

If \( n_1 = 1, l = 1 \), then \( \xi_c(G(w)) = 0 \). 

4. An Illustration

Bipartite graphs have been used in investigating structural features in the areas of molecular biology and chemistry (for example, \([38, 39]\)). We consider here a complete bipartite graph \( K_{m,n} \), where \( m, n > 1 \), with the bipartition \( V_1 \cup V_2 \) of the vertices such that \( V_1 = \{u_1, \ldots, u_m\} \) and \( V_2 = \{v_1, \ldots, v_n\} \). The graph \( K_{m,n} \) is a PWRG G(w) corresponding to the word \( w = a^m b^n \) over the alphabet \{a < b\}.

First, we observe the following facts relating to \( K_{m,n} \):

\[ \xi_c(K_{m,n}) = m \times 2n + n \times 2m = 4mn. \]

The same value is obtained from the formula for the Harary index, namely, \( H(K_{m,n}) = \frac{1}{2}m(m - 1) \times \frac{1}{2} + \frac{1}{2}n(n - 1) \times \frac{1}{2} + \frac{1}{2}mn \)

\[ = \frac{1}{4}(m^2 + n^2 - m - n + 4mn). \]

The same value is obtained from the formula for the eccentric connectivity index, namely, \( \xi_c(K_{m,n}) = 6|w|_{ab} - k|w|_a - n_1|w|_b \), where \( k \) is the number of b's succeeding the
last $a$ and $n_1$ is the number of $a$’s prior to the first $b$ in $G(w)$, so that $k = n, n_1 = m$.

The total eccentricity index of $K_{m,n}$ by direct computation from the definition, is
\[ \zeta(K_{m,n}) = m \times 2 + n \times 2 = 2m + 2n. \] (21)

The same value is obtained from the formula for the total eccentricity index, namely, $\zeta(G(w)) = 3|w| - k - n_1$, where $|w| = |w_a| + |w_b| = m + n$.

The eccentric connectivity coindex of $K_{m,n}$, by direct computation (using the modified expression for the eccentric connectivity coindex given in the proof of Theorem 6), is
\[ \xi(K_{m,n}) = (N - 1) \sum_{u \in V(K_{m,n})} e(u) - \xi(G_{m,n}), \] (22)

where $N$ is the number of vertices in the graph $K_{m,n}$, so that
\[ \xi(K_{m,n}) = (m + n - 1)(m + n) \times 2 - 4mn \]
\[ = 2(m^2 + n^2 - m - n). \] (23)

The same value is obtained from the formula for the eccentric connectivity coindex, namely,
\[ \xi(G(w)) = (|w| - 1)(3|w| - n_1 - k) \]
\[- 6|w|_{ab} + k|w_a| + n_1|w_b| \]
\[ = (m + n - 1)(3(m + n) - m - n) - 6mn \]
\[ = mn + mn = 2(m^2 + n^2 - m - n). \] (24)

5. Conclusion

The distance-based topological indices considered in this study have been extensively investigated by researchers for different classes of graphs, and so we were motivated to study these indices for a recently introduced special class of graphs, called PWRGs. An advantage of this study is that this provides a link between two different areas of research, namely, word combinatorics and graph theory. Specifically, we have obtained expressions for evaluating certain distance-based topological indices for PWRGs [14] of binary core words and established bounds on their values when the vertex set is fixed. It will be of interest to study bounds on these indices when the number of edges is fixed.

Data Availability

The data used to support the findings of this study are included within the article.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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