Certain Distance-based Topological Indices of Parikh Word Representable Graphs

Nobin Thomas
Department of Basic Sciences, Amal Jyothi College of Engineering,
Kanjirappally, Kerala 686 518 India
and
Research scholar, APJ Abdul Kalam Technological University,
Thiruvananthapuram, Kerala 695 016 India

Lisa Mathew
Department of Basic Sciences, Amal Jyothi College of Engineering,
Kanjirappally, Kerala 686 518 India

Sastha Sriram
Department of Mathematics, School of Arts, Science and Humanities,
SASTRA Deemed University, Tanjore, Tamil Nadu 613 401 India

Atulya K. Nagar
School of Mathematics, Computer Science and Engineering
Liverpool Hope University, Liverpool, L16 9JD U.K.

K.G. Subramanian*
School of Mathematics, Computer Science and Engineering,
Liverpool Hope University, Liverpool, L16 9JD U.K.
* Honorary Visiting Professor

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Abstract

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 paper, 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 (see, for example, [8, 16, 22, 23]). 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 [26] and intensively investigated by many researchers (see, for example, [2, 3, 6, 27, 31, 33, 34] 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 [5] and its relationship with the corresponding word and partition was studied in [25].

On the other hand there has been a great interest in various topological indices associated with graphs (see, for example, [1, 13, 14, 21]) due to their application in the area of chemical graph theory [11], 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 (see, for example, [15]) 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 [35], properties of one of the important topological indices, namely, Wiener index and some of its variants related to $PWRG$s of binary words, were studied. In this paper, certain distance-based topological indices of $PWRG$s of binary core words are investigated.

2 Preliminaries

The basic definitions and notations relating to words are as given in [24, 29]. We recall here some of the needed notions.

An ordered alphabet Σ is a set of symbols with an ordering on its symbols. For example, $\Sigma = \{a_1, a_2, \cdots, a_k\}$ 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 Σ is a finite sequence of symbols belonging to Σ. A word w' is a scattered subword or simply called a subword of a word w over Σ if and only if there exist $u_1, u_2, \cdots, u_n$, $u_i \in \Sigma$ for $1 \leq i \leq n$ and words (possibly empty) $v_0, v_1, \cdots, v_n$

over Σ, such that $w' = u_1u_2\cdots u_n,\ w = v_0u_1v_1u_2v_2\cdots v_{n-1}u_nv_n$. The number of occurrences of a word u as a subword of w is denoted by $|w|_u$. For example, in the word $w = aababb$ 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 below with the symbols a and b of ab shown in bold in $aababb$.

$$\mathbf{a}a\mathbf{b}abb, \mathbf{a}aba\mathbf{b}b, \mathbf{a}abab\mathbf{b}, a\mathbf{ab}abb, a\mathbf{a}ba\mathbf{b}b, a\mathbf{a}bab\mathbf{b}, aab\mathbf{ab}b, aab\mathbf{a}b\mathbf{b}.$$

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

Definition 1 *[34] Let $w \in \Sigma^*$. The core of w, denoted by $core(w)$, is the unique word w_0 of w with the smallest possible length such that $w \in b^*w_0a^*$. A word $w \in \Sigma^*$ is called a core word if and only if $core(w) = w$.*

Clearly, a non empty binary word $w \in \Sigma^*$ is a core word if and only if w starts with a and ends with b.

In [5], 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 *[5] 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 $1, 2, \cdots, n$ 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 [5] 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. Fig. 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 $aababab$ is 7 and there are 9 occurrences of the subword ab in $aababab$.

In this paper, we deal with only binary core words and the corresponding $PWRG$s. Also, we note that for a nonempty binary core word of the form $w = a^{n_1}ba^{n_2}b\cdots a^{n_{|w|_b}}b$ 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

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

Note that in the word w, $n_k, 1 \leq k \leq |w|_b$ which is a power of a, indicates that there are n_k vertices labelled 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.

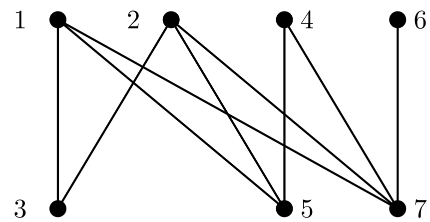

Figure 1: The $PWRG$ of the word $aababab$

3 Distance-based Topological Indices

We consider only simple graphs and for notions related to graphs we refer to [7]. 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 incident at u, is denoted by $deg(u)$. For a given vertex u in a connected graph G, the eccentricity $\epsilon(u)$ is defined as the maximum distance between u and any other vertex in G.

Definition 3 *[19] 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.,*

$$H(G) = \sum_{\{u,v\}\subseteq V(G)} \frac{1}{d(u, v)}.$$

The Harary index [19] of a connected graph is a topological index which has been extensively investigated (see, for example, [10, 36, 37]).

Theorem 3.1 *The Harary index of the $PWRG$ $G(w)$, for $w = a^{n_1}ba^{n_2}b\cdots a^{n_l}b$, $n_1 \geq 1$, $n_k \geq 0$ for $2 \leq k \leq l$, is given by*

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

Proof We consider pairs of vertices (u, v) in the $PWRG$ $G(w)$ corresponding to the word $w = a^{n_1}ba^{n_2}b\dots a^{n_l}b$, with $u, v \in \{1, 2, \cdots, n\}$ 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

as a pair of type 1, 2, 3 and 4 respectively. There are $(n_1 + n_2 + \cdots + n_l)C_2 = |w|_a C_2 = \frac{1}{2}|w|_a(|w|_a - 1)$ pairs of vertices of type 1 and $lC_2 = |w|_b C_2 = \frac{1}{2}|w|_b(|w|_b - 1)$ of type 4 and the distance between each such pair is 2. (Here ${}_nC_r$ is the binomial representing the number of ways of choosing r objects from n objects). There are $ln_1 + (l-1)n_2 + \cdots + n_l = |w|_{ab}$ pairs of vertices of type 2 with distance 1 and $n_2 + 2n_3 + \cdots + (l-1)n_l = |w|_a|w|_b - |w|_{ab}$ pairs of vertices of type 3 with distance 3, since $|w|_{ab} = (n_1 + n_2 + \cdots + n_{|w|_b}) + \cdots + (n_1 + n_2) + n_1$. Hence

$$H(G(w)) = \frac{1}{4}\Big(|w|_a(|w|_a - 1) + |w|_b(|w|_b - 1)\Big) + |w|_{ab} + \frac{1}{3}\Big(|w|_a|w|_b - |w|_{ab}\Big)$$

which yields the required result.

Theorem 3.2 *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 $w = a^{n_1}ba^{n_2}b\cdots a^{n_q}b, n_1 \geq 1$, $n_k \geq 0$ for $2 \leq k \leq l$, is bounded below by*

$$\frac{1}{12}\big(3p^2 + 3q^2 + 4pq + 5p + 5q - 8\big)$$

and above by

$$\frac{1}{4}\big(p^2 + q^2 + 4pq - p - q\big).$$

The bounds are attained on $G(ab^{q-1}a^{p-1}b)$ and $G(a^pb^q)$ respectively.

Proof

Since $G(w)$ is connected, $|w|_{ab} = |E| \geq p + q - 1$ [7]. Also $|w|_{ab} \leq pq$ [26]. Hence from Theorem 3.1, the Harary index of $G(w)$ is

$$\begin{aligned} H(G(w)) &\leq \frac{1}{12}\big(3p^2 + 3q^2 + 12pq - 3p - 3q\big) \\ &= \frac{1}{4}\big(p^2 + q^2 + 4pq - p - q\big) \end{aligned}$$

which is the Harary index of the $PWRG$ $G(a^pb^q)$ and

$$H(G(w)) \geq \frac{1}{12}\big(3p^2 + 3q^2 + 4pq + 5p + 5q - 8\big)$$

which is the Harary index of the $PWRG$ $G(ab^{q-1}a^{p-1}b)$.

Definition 4 *[30] The eccentric connectivity index of a connected graph G with vertex set V, is defined as $\zeta_c(G) = \sum_{v \in V} \epsilon(v)deg(v)$ where $\epsilon(v)$ is the eccentricity of v.*

The total eccentricity index [12] of the graph G is $\zeta(G) = \sum_{v \in V} \epsilon(v)$.

The topological index, namely, eccentric connectivity index, was introduced in [30] and has been widely investigated for different classes of graphs (See, for example, [9, 17, 28, 38] and references therein).

Theorem 3.3 *The eccentric connectivity index of the PWRG $G(w)$, for $w = a^{n_1}ba^{n_2}b \cdots a^{n_l}b, n_1 \geq 1$ is given by*

$$\zeta_c(G(w)) = \begin{cases} 6|w|_{ab} - k|w|_a - n_1|w|_b, \textit{ if } |w|_a > 1 \textit{ and } |w|_b = l > 1 \\ 3|w|_b, \textit{ if } n_1 = 1, n_i = 0, \textit{ for } 1 < i \leq l \textit{ and } l > 1 \\ 3|w|_a, \textit{ if } n_1 > 1 \textit{ and } l = 1 \\ 2, \textit{ if } n_1 = 1, l = 1 \end{cases}$$

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

Proof

Let $G(w)$ be the $PWRG$ corresponding to $w = a^{n_1}ba^{n_2}b \cdots a^{n_l}b$. 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 $G(w)$ representing

(i) a's in the first block $a^{n_1}b$ is $2n_1|w|_b$, as each vertex corresponding to such an a has degree $|w|_b$,

(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

(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,

$$\begin{aligned} \zeta_c(G(w)) &= 2n_1|w|_b + 2k|w|_a + 3(2|w|_{ab} - n_1|w|_b - k|w|_a) \\ &= 6|w|_{ab} - n_1|w|_b - k|w|_a \end{aligned}$$

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. Therefore,

$$\zeta_c(G(w)) = 3|w|_b, \ if \ n_1 = 1 \ and \ n_i = 0, \ 1 < i \leq l$$

Similarly, if $n_1 > 1$ and $l = 1$, $w = a^{n_1}b$ 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 $G(w)$, for $w = a^{n_1}ba^{n_2}b\cdots a^{n_l}b, n_1 \geq 1$ is given by*

$$\zeta(G(w)) = \begin{cases} 3|w| - k - n_1, \text{ if } |w|_a > 1 \text{ and } l > 1 \\ 2|w|_b + 1, \text{ if } n_1 = 1, n_i = 0, \text{ for } 1 < i \leq l \text{ and } l > 1 \\ 2|w|_a + 1, \text{ if } n_1 > 1 \text{ and } l = 1 \\ 2, \text{ if } n_1 = 1, l = 1 \end{cases}$$

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

Theorem 3.4 *The eccentric connectivity index $\zeta_c(G(w))$ of a PWRG $G(w) = (V_1 \cup V_2, E)$ with $|V_1| = |w|_a = p > 1, |V_2| = |w|_b = q > 1$ for the word $w = a^{n_1}ba^{n_2}b\cdots a^{n_q}b, n_1 \geq 1,\ n_i \geq 0$ for $2 \leq i \leq l$, is bounded above by ζ_c^{max} and below by ζ_c^{min} where*

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

and

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

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

Proof Since $|w|_a = p > 1, |w|_b = q > 1$, using Theorem 3.3, the eccentric connectivity index $\zeta_c(G(w)) = 6|w|_{ab} - k|w|_a - n_1|w|_b$, will be a maximum if $|w|_{ab}$ is as large as possible while n_1 and k are as small as possible. (Here k is the number of b's succeeding the last a in w.) It is known [27] that for a binary word w,$|w|_{ab} \leq pq$ when $|w|_a = p, |w|_b = q$. The word a^pb^q has the maximum number pq of subwords ab and so the eccentric connectivity index of the $PWRG$ corresponding to this word is maximum but only when $p + q \leq 6$. We note that $p > 1$, and $q > 1$ and the word w is a core word by the hypothesis. When $p + q > 6$, it can be verified that this word fails to provide the maximum eccentric connectivity index for the corresponding $PWRG$ due to the fact that all the vertices in the $PWRG$ of a^pb^q have only eccentricity 2. When $|w|_{ab} = pq - 1$, which is the largest number nearer to the maximum pq, the word $a^{p-1}bab^{q-1}$ has $pq - 1$ subwords ab while the vertices in the $PWRG$ corresponding to the first b and the next a in this word, have eccentricity 3 and degrees $p - 1$ and $q - 1$ respectively. The eccentric connectivity index of the $PWRG$ corresponding to this word $a^{p-1}bab^{q-1}$ is maximum when $p+q \geq 6$ but only when $2pq - 8p - 8q + 24 \leq 0$. When $p + q > 6$ and $2pq - 8p - 8q + 24 > 0$, it can be verified that the word $a^{p-1}bab^{q-1}$ fails to provide the maximum eccentric connectivity index for the corresponding $PWRG$. On the other hand the word $aba^{p-2}b^{q-2}ab$ has the minimum value 1 for n_1 and k and has as many $a's$ as possible to the left and as many $b's$ as possible to the right of the word, thus providing maximum degrees for the vertices in the $PWRG$ corresponding to the $a's$ and $b's$ in $a^{p-2}b^{q-2}$ which have eccentricity 3. In fact, more formally, for $w = a^{n_1}ba^{n_2}b\cdots a^{n_q}b$,$n_1 \geq 1, q > 1$, $n_1 + n_2 + \cdots n_q = p > 1$, we can show that

$$\zeta_c(G(w)) = 6pq - n_1q - 3qn_q + 2p - 3(n_1 + 3n_2 + 5n_3 + \cdots + (2q-3)n_{q-1} + (q-1)n_q).$$

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 $w_1 = a^pb^q, w_2 = a^{p-1}bab^{q-1}$ or $w_3 = aba^{p-2}b^{q-2}ab$ whose corresponding $PWRG$s $G(w_1), G(w_2), G(w_3)$ have their eccentric connectivity indices as $\eta_1 = 4pq, \eta_2 = 4pq + p + q - 6, \eta_3 = 6pq - 7p - 7q + 18$ respectively. Note that $\eta_1 \geq \eta_2$ when $p + q \leq 6$ while the expression $2pq - 8p - 8q + 24$ is the difference $\eta_3 - \eta_2$. Hence the maximum value is attained on $G(a^pb^q)$ when $p + q \leq 6$, on $G(a^{p-1}bab^{q-1})$ when $p + q \geq 6, 2pq - 8p - 8q + 24 \leq 0$ and on $G(aba^{p-2}b^{q-2}ab)$ when $p + q > 6$ and $2pq - 8p - 8q + 24 > 0$.
On the other hand, for $p > 1, q > 1$, $\zeta_c(G(w))$ is minimum when $|w|_{ab}$ is minimum and this happens for $w = a^{n_1}b^{q-k}a^{p-n_1}b^k$ with $|w|_{ab} = n_1q + pk - n_1k$ minimum when $n_1 = k = 1$. Hence the minimum value $5p + 5q - 6$ of $\zeta_c(G(w))$ is attained on $G(ab^{q-1}a^{p-1}b)$.

Theorem 3.5 *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 $w = a^{n_1}ba^{n_2}b\cdots a^{n_q}b$, $n_1 \geq 1$, $n_i \geq 0$ 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 $|u|_a = p - 2, |u|_b = q - 2$. In particular it is achieved on $G(ab^{q-1}a^{p-1}b)$. The lower bound is achieved on $G(a^pb^q)$.*

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

Yet another topological index, called eccentricity connectivity coindex [4, 18] of a connected graph, is defined as the eccentricity sum of all non-adjacent vertex pairs in the graph. We consider this index here for $PWRG$s.

Definition 5 *[4, 18] The eccentric connectivity coindex $\overline{\zeta_c}(G)$ of a connected graph G with edge set $E(G)$ is defined as*

$$\overline{\zeta_c}(G) = \sum_{uv \notin E(G)} (\epsilon(u) + \epsilon(v))$$

where $\epsilon(x)$ is the eccentricity of the vertex x of G.

Theorem 3.6 *The eccentric connectivity coindex $\overline{\zeta_c}(G(w))$ of the PWRG $G(w)$, for $w = a^{n_1}ba^{n_2}b\cdots a^{n_l}b, n_1 \geq 1$, $n_k \geq 0$ for $2 \leq k \leq l$ is given by*

$$\overline{\zeta_c}(G(w)) = \begin{cases} (|w|-1)(3|w|-n_1-k) - 6|w|_{ab} + k|w|_a + n_1|w|_b, \\ \qquad\qquad\qquad\qquad \textit{if } |w|_a > 1, l > 1 \\ 2|w|_b(|w|_b - 1), \quad \textit{if } n_1 = 1, n_i = 0, 1 < i \leq l, l > 1 \\ 2|w|_a(|w|_a - 1), \quad \textit{if } n_1 > 1, l = 1 \\ 0, \quad \textit{if } n_1 = 1, l = 1. \end{cases}$$

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

Proof It has been shown [4, 18] that $\overline{\zeta_c}(G) = \sum_{u\in V(G)} \epsilon(u)(n-1-deg(u))$ which can be written as $\overline{\zeta_c}(G) = (n-1)\sum_{u\in V(G)} \epsilon(u) - \zeta^c(G)$ 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,

$$\overline{\zeta_c}(G(w)) = (|w|-1)(3|w|-n_1-k) - 6|w|_{ab} + k|w|_a + n_1|w|_b.$$

Now, if $n_1 = 1, n_i = 0$ for $1 < i \leq l$ and $l > 1$, then the vertex corresponding to a is of eccentricity one and the remaining vertices are of eccentricity two.
Therefore, $\overline{\zeta_c}(G(w)) = 2|w|_b(|w|_b - 1)$.
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 $\overline{\zeta_c}(G(w)) = 2|w|_a(|w|_a - 1)$.
If $n_1 = 1, l = 1$, then $\overline{\zeta_c}(G(w)) = 0$.

4 An Illustration

Bipartite graphs have been used in investigating structural features in the areas of molecular biology and chemistry (see, for example, [20, 32]). We consider here a complete bipartite graph $K_{m,n}, m, n > 1$, with the bipartition $V_1 \cup V_2$ of the vertices such that $V_1 = \{u_1, \cdots, u_m\}$ and $V_2 = \{v_1, \cdots, n_n\}$. 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 $K_{m,n}$.

(i) For $1 \leq i, j \leq m, 1 \leq r, s \leq n$, $u_i, u_j \in V_1, i \neq j$, and $v_r, v_s \in V_2, r \neq s$, we have $d(u_i, u_j) = d(v_r, v_s) = 2, d(u_i, v_r) = 1$, $\epsilon(u_i) = \epsilon(v_r) = 2$.

(ii) In the graph $K_{m,n}, m, n > 1$, there are $\frac{1}{2}m(m-1)$ unordered pairs of vertices $(u_i, u_j), i \neq j$, $\frac{1}{2}n(n-1)$ unordered pairs of vertices $(v_r, v_s), r \neq s$, and mn unordered pairs of vertices (u_i, v_r).

(iii) The degree of each vertex $u_i, 1 \leq i \leq m$ is $deg(u_i) = n$ and the degree of each vertex $v_r, 1 \leq r \leq n$ is $deg(v_r) = m$.

We now illustrate the computation of the topological indices considered in the earlier sections, both directly from the definition and from the formulas in Theorems 3.1, Theorem 3.3 and Remark 1.

The Harary index of $K_{m,n}$, by direct computation from the definition, is

$$H(K_{m,n}) = \frac{1}{2}m(m-1)\times\frac{1}{2}+\frac{1}{2}n(n-1)\times\frac{1}{2}+mn = \frac{1}{4}\left(m^2+n^2+-m-n+4mn\right).$$

The same value is obtained from the formula for the Harary index, namely, $H(G(w)) = \frac{1}{12}\Big(3|w|_a(|w|_a-1)+3|w|_b(|w|_b-1)+8|w|_{ab}+4|w|_a|w|_b\Big)$ since $|w|_a = m, |w|_b = n, |w|_{ab} = mn$.

The eccentric connectivity index of $K_{m,n}$, by direct computation from the definition, is

$$\zeta_c(K_{m,n}) = m \times 2n + n \times 2m = 4mn.$$

The same value is obtained from the formula for the eccentric connectivity index, namely, $\zeta_c(G(w)) = 6|w|_{ab} - k|w|_a - n_1|w|_b$ where $k =$ the number of $b's$ succeeding the last a and $n_1 =$ 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

$$\zeta(K_{m,n}) = m \times 2 + n \times 2 = 2m + 2n.$$

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 3.6), is

$$\overline{\zeta_c}(K_{m,n}) = (N-1)\sum_{u\in V(K_{m,n})}\epsilon(u) - \zeta^c(K_{m,n})$$

where N is the number of vertices in the graph $K_{m,n}$ so that

$$\overline{\zeta_c}(K_{m,n}) = (m+n-1)(m+n)\times 2 - 4mn = 2(m^2+n^2-m-n).$$

The same value is obtained from the formula for the eccentric connectivity coindex, namely,

$$\overline{\zeta_c}(G(w)) = (|w|-1)(3|w|-n_1-k) - 6|w|_{ab} + k|w|_a + n_1|w|_b$$

$$= (m+n-1)(3(m+n)-m-n) - 6mn + nm + mn) = 2(m^2+n^2-m-n).$$

5 Conclusion

The distance-based topological indices considered in this paper 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 $PWRG$s. 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 $PWRG$s [5] 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.

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6 Conflicts of Interest

The authors declare that there is no conflict of interest regarding the publication of this article.

References

[1] A. Aslam, J. L. G. Guirao, S. Ahmad and W. Gao, "Topological indices of line graph of subdivision graph of complete bipartite graphs", *Applied Mathematics and Information Sciences*, vol. 11, no. 6, pp. 1631–1636, 2017.

[2] A. Atanasiu, "Binary amiable words", *International Journal of Foundations of Computer Science*, vol. 18, no. 02, pp. 387–400, 2007.

[3] A. Atanasiu, R. Atanasiu, and I. Petre, "Parikh matrices and amiable words", *Theoretical Computer Science,* vol. 390, no.1, pp. 102–109, 2008.

[4] M. Azari, "Eccentric connectivity coindex under graph operations", *Journal of Applied Mathematics and Computing*, vol. 62, pp. 23–35, 2020.

[5] S. Bera, K. Mahalingam, "Structural properties of word representable graphs", *Mathematics in Computer Science*, vol. 10, no. 2, pp. 209–222, 2016.

[6] S. Bera, K. Mahalingam, and K. G. Subramanian, "Properties of Parikh matrices of binary words obtained by an extension of a restricted shuffle operator, *International Journal of Foundations of Computer Science,* vol. 29, pp. 403–414, 2009.

[7] G. A. Bondy, U. S. R. Murty, *Graph Theory with Applications*, North-Holland, 1982.

[8] A. Collins, S. Kitaev, and V. Lozin, "New results on word-representable graphs", *Discrete Applied Mathematics*, vol. 216, pp. 136–141, 2017.

[9] P. Dankelmann, M.J. Morgan, S. Mukwembi, and H. C. Swart, "On the eccentric connectivity index and Wiener index of a graph", *Quaestiones Mathematicae*, vol. 37, no. 1, pp. 39-47, 2014.

[10] K. C. Das, K. Xu, I. N. Cangul, A.S. Cevik, and A. Graovac," On the Harary index of graph operations", *Journal of Inequalities and Applications*, Article no. 339, 2013.

[11] M. Diudea, *Basic Chemical Graph Theory*, In: Multi - shell Polyhedral Clusters . Carbon Materials : Chemistry and Physics, vol. 10, Springer, 2018.

[12] K. Fathalikhani, H. Faramarzi, H. Yousef, H. Azari, "Total eccentricity of some graph operations", *Electronic Notes in Discrete Mathematics*, vol. 45, pp. 125–131, 2014.

[13] W. Gao, Z. Iqbal, M. Ishaq, R. Sarfraz, M. Aamir and A. Aslam, "On eccentricity based topological indices study of class of Porphyrin-cored dendrimers", *Biomolecules*, vol. 8, article 71, 2018.

[14] W. Gao, Z. Iqbal, M. Ishaq, A. Aslam, R. Sarfraz, "Topological aspects of dendrimers via distance based descriptors", IEEE access, vol. 7, pp. 35619–35630, 2019.

[15] I. Gutman, and O. Polansky, *Mathematical concepts in Organic Chemistry*, Springer -Verlag, 1986.

[16] M. M. Halldórsson, S. Kitaev, and A. Pyatkin, "Graphs Capturing Alternations in Words", In: Gao Y., Lu H., Seki S., Yu S. (eds) Developments in Language Theory. DLT 2010, *Lecture Notes in Computer Science*, Springer, Berlin, vol. 6224, pp. 436–437, 2010.

[17] R. S. Haoer, K. A. Atan, A. M. Khalaf and R. Hasni, "Eccentric connectivity index of unicyclic graphs with application to cycloalkanes," 2015 International Conference on Research and Education in Mathematics (ICREM7), Kuala Lumpur, Malaysia, pp. 211-214, 2015.

[18] H. Hua, and Z. Miao, "The total eccentricity sum of non-adjacent vertex pairs in graphs", *Bulletin of the Malaysian Mathematical Sciences Society,* vol. 42, pp. 947–963, 2019.

[19] O. Ivanciuc, T-S. Balaban, and A. T. Balaban, "Design of topological indices. part 4. reciprocal distance matrix, related local vertex invariants and topological indices", *Journal of Mathematical Chemistry,* vol. 12, pp. 309–318, 1993.

[20] P. Iyer and J. Bajorath, “Mechanism-based bipartite matching molecular series graphs to identify structural modifications of receptor ligands that lead to mechanism hopping”, *Med. Chem. Commun.,* vol. 3, pp. 441—448, 2012.

[21] S. M. Kang, Z. Iqbal, M. Ishaq, R. Sarfraz, A. Aslam and W. Nazeer, “On eccentricity-based topological indices and polynomials of phosphorus-containing dendrimers”, *Symmetry*, vol. 10, article 237, 2018.

[22] S. Kitaev, and V. Lozin, *Words and Graphs,* Springer, vol. 17, 2015.

[23] S. Kitaev, P. Salimov, C. Severs, and H. Ulfarsson, “Word-representability of line graphs,” *Open Journal of Discrete Mathematics*, vol. 1, pp. 96–101, 2011.

[24] M. Lothaire, *Combinatorics on Words*, Cambridge Mathematical Library, Cambridge university Press, 1997.

[25] L. Mathew, N. Thomas, S. Bera, and K. G. Subramanian, “Some results on Parikh word representable graphs and partitions”, *Advances in Applied Mathematics*, vol. 107, pp. 102–115, 2019.

[26] A. Mateescu, A. Salomaa, K. Salomaa, and S. Yu, “A sharpening of the Parikh mapping,” *RAIRO - Theoretical Informatics and Applications*, vol. 35, no. 6, pp. 551–564, 2001.

[27] A. Mateescu, and A. Salomaa, “Matrix indicators for subword occurrences and ambiguity”, *International Journal of Foundations of Computer Science,* vol. 15, no. 02, pp. 277–292, 2004.

[28] M. J. Morgan, S. Mukwembi, and H. C. Swart, “On the Eccentric Connectivity Index of a Graph”, *Discrete Mathematics*, vol. 311, n0. 13, pp. 1229–1234, 2011.

[29] G. Rozenberg, and A. Salomaa, *Handbook of formal languages*, Springer, 1997.

[30] V. Sharma, R. Goswami, and A. Madan, “Eccentric connectivity index: A novel highly discriminating topological descriptor for structure-property and structure-activity studies”, *Journal of chemical information and computer sciences*, vol. 37, pp. 273–282, 1997.

[31] K. G. Subramanian, A. Miin Huey, and A. Nagar, “On Parikh matrices”, *International Journal of Foundations of Computer Science,* vol. 20, pp. 211–219, 2009.

[32] W.R. Taylor, “Protein Structure Comparison Using Bipartite Graph Matching and Its Application to Protein Structure Classification”, *Molecular & Cellular Proteomics,* vol. 1(4), pp. 334—339, 2002.

[33] W. C. Teh, "On core words and the Parikh matrix mapping," *International Journal of Foundations of Computer Science*, vol. 26, no. 01, pp. 123–142, 2015.

[34] W. C. Teh, and K. H. Kwa, "Core words and Parikh matrices", *Theoretical Computer Science*, vol. 582, pp. 60–69, 2015.

[35] N. Thomas, L. Mathew, S. Sriram, and K. G. Subramanian, "Wiener-type Indices of Parikh Word Representable Graphs", *Ars Mathematica Contemporanea*, (Accepted for publication).

[36] K. Xu, and K. C. Das, "On Harary Index of Graphs", *Discrete Applied mathematics*, vol. 159, no. 15, pp. 1631–1640, 2011.

[37] B-H. Xing, G-D. Yu, L-X. Wang, and J. Cao, "The Harary Index of All Unicyclic Graphs with Given Diameter", *Discrete Dynamics in Nature and Society*, vol. 2018, Article ID 3957023, 6 pages, 2018.

[38] B. Zhou, and Z. Du, "On Eccentric Connectivity Index", *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 63, pp. 181–198, 2010.