RESEARCH ARTICLE
doi: 10.2306/scienceasia1513-1874.2024.009

ScienceAsia 50 (3): 2024: ID 2024009: **1–6**

Existence and non-existence of total eccentric graphical intervals

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Received 11 Apr 2022, Accepted 24 Aug 2023
Available online 23 Jan 2024

ABSTRACT: A topological index is a numerical invariant which depicts the properties of molecules in accordance to their chemical structure. For a given integer $n > 0$, if a graph G exists with a total eccentric index of $\zeta(G) = n$, then "n" is said to be total eccentric graphical, which is kind of an inverse problem for topological indices. An (integer) interval $[\alpha, \beta]$ is called p-total eccentric (free) interval if for all $n \in [\alpha, \beta]$ there exists a (no) graph $G(p, q)$ with $\zeta(G) = n$. In this article, we determine several results for the existence and non-existence of total eccentric graphical intervals for graphs G on p vertices.

KEYWORDS: eccentricity, total eccentric index, p-total eccentric interval, p-total eccentric free intervals

MSC2020: 05C12 05C38 92E10

INTRODUCTION

Preliminaries

Molecular graph theory is one of the prominent areas in mathematical chemistry. The chemical structures are converted into graph theory invariants by considering atoms as vertices and edges as covalent bonds between the atoms. In the field of computational chemistry as well as physical chemistry, these methods are used to predict molecular properties and test theoretical concepts using computational methods. With the help of topological indices, QSAR/QSPR studies [1] are rapidly growing by applying mathematical principles to infer the characteristics and biological interactions of diverse chemical substances. This study is particularly useful when the chemical substance is unavailable and when predicting molecular properties that are either difficult to find or may pose health risks.

A topological index is a one-of-a-kind real value that could be assigned to molecular graphs via a function or mapping. Usually, it is a unique real number related to the molecular graph's structure. The task of creating a chemical structure (a graph) with a given molecular index (if it exists) is known as the "inverse problem" of the *molecular index*.

Definition 1 Total eccentric index of $G = \zeta(G) = \sum_{x \in V(G)} e(x)$ where $e(x) = \max_{y \in V(G)} d(x, y)$.

Definition 2 If a graph G exists for a given order p with $\zeta(G) = n$ for all $n \in [\alpha, \beta]$ then the integer interval $[a, b]$ is called p-total eccentric interval.

Definition 3 If there exists no graph G for a given order p with $\zeta(G) = n$ for all $n \in [\alpha, \beta]$ then the integer interval $[a, b]$ is called p-total eccentric free interval.

Literature survey

In [2], Goldman et al initially studied the inverse problems and discovered that this could be used in building the data base for drug development in computer chemistry. Chemical compounds with desired structure and properties are uncovered, developed, and enhanced using computer-aided drug discovery (CADD), as discussed in [3, 4]. Computational chemists could use the inverse problem to design or study a chemical structure with a specific chemical and biological properties, which are studied in [5–9]. As a result of their widespread use and modern technological capabilities, many indices have been developed and their mathematical and chemical parameters evaluated. Many eccentricity-based indices have been developed; the formulation of safe anti-HIV pharmaceuticals is one of their significant contributions [5]. The total eccentric index is the over all sum of the eccentricities of a graph [10], and it is being researched further for its potential applications in a variety of fields, discussed in [11–15].

Methodology

The first and most popular distance-based topological index was the Wiener index, which was introduced in [16]. As a result of its applications in numerous disciplines [17–19], many other topological indices of chemical graphs have been introduced and studied [20]. The inverse problem of finding a graph with given order p, whose Wiener index $n \in [\alpha, \beta]$ is introduced in [21]. The authors established various intervals and free intervals for the well-known Weiner index. Also, they proved $[\binom{p}{2}, (p-1)^2]$ and $[\binom{p}{2}, (p-1)^2 + k(p-3)]$ are p-Wiener intervals, and

$\left[\frac{p^2-7p+24}{6}, \frac{p^2-p-6}{6}\right]$ is a p-Wiener free interval. As a result of these findings, we enhanced this strategy for the total eccentric index and established certain p-eccentric graphical intervals and p-eccentric graphical free intervals for total eccentric index. In addition, we find a relationship between the total eccentric index of a graph G and $G-e$. For graph theoretical definitions and terminologies, we follow [18, 22–24].

Theorem 1 ([2]) *For any path P with y edges and $y+1$ vertices,*

$$\zeta(P)=\begin{cases}\frac{3}{4}y^2+y, & \text{if } y \text{ is even}\\ \frac{3}{4}y^2+y+1/4, & \text{if } y \text{ is odd.}\end{cases}$$

MAIN RESULT

Theorem 2 *For each k, $2 \leqslant k \leqslant p-2$, $\left[\left\lceil \frac{(3p+k)(p-k)-4k+4}{4}\right\rceil, \left\lceil \frac{(3p+k)(p-k)}{4}\right\rceil\right]$ is a p-total eccentric interval and all these intervals are mutually disjoint.*

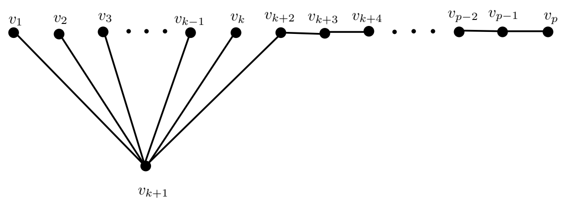

Fig. 1 The constructed graph G.

Proof: Let G be a graph whose vertex set is $\{v_1, v_2, \dots, v_p\}$ and the edge set is $\{v_j v_{k+1} : 1 \leqslant j \leqslant k\} \cup \{v_j v_{j+1} : k+1 \leqslant j < p\}$. Fig. 1 depicts the graph that is constructed. In the graph G,

$$e(v_j)=\begin{cases}p-k, & \text{for } 1 \leqslant j \leqslant k\\ p-j, & \text{for } k+1 \leqslant j \leqslant k+\lfloor\frac{p-k}{2}\rfloor\\ j-k, & \text{for } k+\lfloor\frac{p-k}{2}\rfloor+1 \leqslant j \leqslant p.\end{cases}$$

Now

$$\sum_{j=1}^{k} e(v_j)=\sum_{j=1}^{k}(p-k)=k(p-k),$$

$$\begin{aligned}\sum_{j=k+1}^{k+\lfloor\frac{p-k}{2}\rfloor} e(v_j) &= \sum_{j=k+1}^{k+\lfloor\frac{p-k}{2}\rfloor}(p-j)\\ &= p-(k+1)+p-(k+2)+\cdots+p-(k+\lfloor\frac{p-k}{2}\rfloor)\\ &= p-(k+1)+p-(k+2)+\cdots+p-(k+\lfloor\frac{p-k}{2}\rfloor)\\ &= \lfloor\frac{p-k}{2}\rfloor\Big(p-k-\frac{1}{2}\big(\lfloor\frac{p-k}{2}\rfloor+1\big)\Big)\end{aligned}$$

and

$$\begin{aligned}\sum_{j=k+\lfloor\frac{p-k}{2}\rfloor+1}^{p} e(v_j) &= \sum_{j=k+\lfloor\frac{p-k}{2}\rfloor+1}^{p}(j-k)\\ &= \big(k+\lfloor\frac{p-k}{2}\rfloor+1-k\big)+\big(k+\lfloor\frac{p-k}{2}\rfloor+2-k\big)\\ &\quad+\cdots+(p-k)\\ &= \big(p-k-\lfloor\frac{p-k}{2}\rfloor\big)\big(\lfloor\frac{p-k}{2}\rfloor\big)\\ &\quad+\frac{1}{2}\big(p-k-\lfloor\frac{p-k}{2}\rfloor\big)\big(p-k-\lfloor\frac{p-k}{2}\rfloor+1\big)\\ &= \big(p-k-\lfloor\frac{p-k}{2}\rfloor\big)\big(\frac{1}{2}\lfloor\frac{p-k}{2}\rfloor+\frac{p-k+1}{2}\big)\end{aligned}$$

Hence, the total eccentricity of G is,

$$\begin{aligned}\zeta(G) &= \sum_{j=1}^{p} e(v_j)\\ &= \left\lfloor\frac{p-k}{2}\right\rfloor(p-k-1)-\left\lfloor\frac{p-k}{2}\right\rfloor^2+\frac{(p-k)(p+k+1)}{2}\\ &= \begin{cases}\frac{(p-k)(3p+k)}{4}, & \text{if } p-k \text{ is even}\\ \frac{(3p+k)(p-k)+1}{4}, & \text{if } p-k \text{ is odd}\end{cases}\\ &= \left\lceil\frac{(3p+k)(p-k)}{4}\right\rceil.\end{aligned}$$

Let G_1 be the graph obtained from G by joining the vertex v_1 with $v_2, v_3, \dots, v_k$ and v_{k+2}. In G_1, the eccentricity of v_1 is decreased by 1, and the eccentricity of $V(G)-\{v_1\}$ remains the same as in G. This implies that $\zeta(G_1)=\zeta(G)-1=\left\lceil\frac{(3p+k)(p-k)}{4}\right\rceil-1$.

Let G_2 be the graph obtained from G_1 by joining the vertex v_2 with the vertices $v_3, v_4, \dots, v_k$ and v_{k+2}. In G_2, the eccentricity of v_2 is decreased by 1, and the eccentricity of $V(G_1)-\{v_2\}$ remains the same as in G_1. This implies that $\zeta(G_2)=\zeta(G_1)-1=\zeta(G)-2=\left\lceil\frac{(3p+k)(p-k)}{4}\right\rceil-2$.

This process is repeated up to v_{k-1} and the graph G_{k-1}, obtained from G_{k-2} by joining v_{k-1} with v_k and v_{k+2}, has a total eccentric index $\zeta(G_{k-1})=\lceil\frac{(3p+k)(p-k)}{4}\rceil-(k-1)=\lceil\frac{(3p+k)(p-k)-4k+4}{4}\rceil$.

Hence, $\left[\left\lceil\frac{(3p+k)(p-k)-4k+4}{4}\right\rceil, \left\lceil\frac{(3p+k)(p-k)}{4}\right\rceil\right]$ is a p-total eccentric interval for each $k, 2 \leqslant k \leqslant p-2$. Denote this p-total eccentric interval as $[A_k, B_k]$, $2 \leqslant k \leqslant p-2$. Take $k=p-i$ and denote the p-total eccentric interval corresponding to $k=p-i$ as $[A'_i, B'_i]$. Then for $2 \leqslant i \leqslant p-2$, $[A'_i, B'_i]=\left[\left\lceil\frac{(4p-i)i-4p+4i+4}{4}\right\rceil, \left\lceil\frac{(4p-i)i}{4}\right\rceil\right]$ and these intervals are mutually exclusive if $A'_{i+1}-B'_i>0$. That is, $[A'_i, B'_i]$ and $[A'_{i+1}, B'_{i+1}]$ are not the overlapped intervals in the real line $\mathbb{R}^+$.

Case(i): i is even

$$\begin{aligned} A'_{i+1} &= \Big\lceil \frac{(4p-i-1)(i+1)-4p+4i+8}{4} \Big\rceil \\ &= \Big\lceil \frac{4pi-i^2}{4} + \frac{2i+7}{4} \Big\rceil \\ &= \frac{4pi-i^2}{4} + \frac{i+4}{2} \quad \text{and} \quad B'_i = \frac{(4p-i)i}{4} \end{aligned}$$

$$\begin{aligned} \text{Then} \quad A'_{i+1} - B'_i &= \frac{4pi-i^2}{4} + \frac{i+4}{2} - \Big(\frac{4pi-i^2}{4}\Big) \\ &= \frac{i}{2} + 2 > 0. \end{aligned}$$

Case(ii): i is odd

$$\begin{aligned} A'_{i+1} &= \Big\lceil \frac{(4p-i-1)(i+1)-4p+4i+8}{4} \Big\rceil \\ &= \Big\lceil p(i+1)-p+i+2-\frac{(i+1)^2}{4} \Big\rceil \\ &= p(i+1)-p+i+2-\frac{(i+1)^2}{4} \\ \text{and} \quad B'_i &= \lceil pi - \frac{i^2}{4} \rceil \\ &= \lceil pi - \frac{(i-1)^2}{4} - \frac{(i-1)}{2} \rceil \\ &= pi - \frac{(i-1)^2}{4} - \frac{(i-1)}{2} \end{aligned}$$

$$\text{Then} \quad A'_{i+1} - B'_i = 2 + \frac{i-1}{2} > 0.$$

Hence, all these intervals are mutually disjoint, and for each k in $2 \leqslant k \leqslant p-2$, the interval $\Big[\Big\lceil \frac{(3p+k)(p-k)-4k+4}{4} \Big\rceil, \Big\lceil \frac{(3p+k)(p-k)}{4} \Big\rceil\Big]$ is a p-total eccentric interval. □

Theorem 3 *For any $p \geqslant 5$, $\Big[\Big\lfloor \frac{3p^2-4p-3}{4} \Big\rfloor + 1, \Big\lfloor \frac{3p^2-2p}{4} \Big\rfloor - 1\Big]$ is a p-total eccentric free interval.*

Proof: Let G_i be a graph obtained from a path $v_1 v_2 \cdots v_{p-1}$ by attaching a pendent vertex v_p to a vertex v_i, for some i, $2 \leqslant i \leqslant \lfloor \frac{p}{2} \rfloor$.

Case(i): p is odd. The eccentricity of the vertices of G_i are

$$e(v_j) = \begin{cases} p-1-j & \text{for } 1 \leqslant j \leqslant \frac{p-1}{2} \\ e(v_{p-j}) & \text{for } \frac{p+1}{2} \leqslant j \leqslant p-1 \end{cases}$$
$$e(v_p) = p - i.$$

and

$$\begin{aligned} \zeta(G_i) &= \sum_{j=1}^{p} e(v_j) = 2 \sum_{j=1}^{\frac{p-1}{2}} (p-1-j) + p - i \\ &= 2\Big[\frac{p-1}{2}(p-1) - (1+2+3+\cdots+\frac{p-1}{2})\Big] + p - i \\ &= \frac{3p^2-8p+5}{4} + p - i \\ &= \frac{3p^2-4p+5}{4} - i. \end{aligned}$$

Case(ii): p is even. The eccentricity of the vertices of G_i are

$$e(v_j) = \begin{cases} p-1-j & \text{for } 1 \leqslant j \leqslant \frac{p}{2}-1 \\ \frac{p-2}{2} & \text{for } j = \frac{p}{2} \\ e(v_{p-j}) & \text{for } \frac{p}{2}+1 \leqslant j \leqslant p-1 \end{cases}$$
$$e(v_p) = p - i.$$

and

$$\begin{aligned} \zeta(G_i) &= \sum_{j=1}^{p} e(v_j) = 2 \sum_{j=1}^{\frac{p}{2}-1} (p-1-j) + \frac{p-2}{2} + p - i \\ &= 2\Big[(\frac{p}{2}-1)(p-1) - (1+2+3+\cdots+(\frac{p}{2}-1))\Big] + \frac{p-2}{2} + p - i \\ &= \frac{3p^2-8p+4}{4} + p - i \\ &= \frac{3p^2-4p+4}{4} - i. \end{aligned}$$

Hence, $\zeta(G_i) = \Big\lfloor \frac{3p^2-4p+5}{4} \Big\rfloor - i$ for $2 \leqslant i \leqslant \lfloor \frac{p}{2} \rfloor$. $\zeta(G_i)$ attains maximum for $i = 2$, that is, i is minimum. Among the trees T on p vertices, $\zeta(T)$ is maximum when T is a path, and the next maximum is obtained from the graph structure having p vertices, which is G_2. If we add more edges to the graph G_2, then the resultant graph's total eccentric index is less than $\zeta(G_2)$. Hence, the result follows. □

Remark 1 For the intervals given in Theorem 3, if $p = 3$ and $p = 4$, the free intervals are $[4, 4]$ and $[9, 9]$ respectively.

Theorem 4 *For any $p \geqslant 4$, $\Big[\Big\lfloor \frac{3p^2-6p+7}{4} \Big\rfloor, \Big\lfloor \frac{3p^2-4p-3}{4} \Big\rfloor\Big]$ is a p-total eccentric interval.*

Proof: From the graph G_i constructed in the proof of Theorem 3, it is observed that $\zeta(G_i) = \zeta(G_{i-1}) - 1 = \zeta(G_2) - (i-2)$, for $3 \leqslant i \leqslant \lfloor \frac{p}{2} \rfloor$. Hence, $\zeta(G_i)$ is minimum when $i = \lfloor \frac{p}{2} \rfloor$, and the minimum value is $\zeta(G_2) - \big(\lfloor \frac{p}{2} \rfloor - 2\big) = \lfloor \frac{3p^2-6p+7}{4} \rfloor$. Hence, the result follows. □

Remark 2 The graph G_2 constructed in Theorem 3 is isomorphic to the graph G constructed in Theorem 2 when $k = 2$. Hence, the upper bounds of both intervals in Theorem 2 and Theorem 4 coincide with each other. The interval $\left[\left\lfloor \frac{3p^2-6p+7}{4}\right\rfloor, \left\lfloor \frac{3p^2-4p-3}{4}\right\rfloor\right]$ is of length $\lfloor \frac{p-2}{2} \rfloor$, and the interval $[A_2, B_2]$ is of length 2. As a result, for all $p \geqslant 6$, $[A_2, B_2]$ is contained in $\left[\left\lfloor \frac{3p^2-6p+7}{4}\right\rfloor, \left\lfloor \frac{3p^2-4p-3}{4}\right\rfloor\right]$. Also, the intervals $[A_3, B_3]$ and $\left[\left\lfloor \frac{3p^2-6p+7}{4}\right\rfloor, \left\lfloor \frac{3p^2-4p-3}{4}\right\rfloor\right]$ are disjoint.

Theorem 5 $\left[\left\lfloor \frac{3p^2-14p}{4}\right\rfloor + p + 4, \left\lfloor \frac{3p^2-14p}{4}\right\rfloor + 2p - 2\right]$ *is a p-total eccentric interval for $p \geqslant 8$.*

Proof: Let G be a graph obtained from a path v_1, v_2, $v_3, \ldots, v_{p-2}$ on $p-2$ vertices by attaching a vertex v_{p-1} at v_i, for some i, $2 \leqslant i \leqslant \lceil \frac{p-2}{2} \rceil$ and a vertex v_p at v_j, for some j, $\lceil \frac{p-2}{2} \rceil + 1 \leqslant j \leqslant p-3$. In the graph G,

$$\begin{aligned} e(v_k) &= \begin{cases} p-2-k & \text{for } 1 \leqslant k \leqslant \lceil \frac{p-2}{2} \rceil \\ k-1 & \text{for } \lceil \frac{p-2}{2} \rceil + 1 \leqslant k \leqslant p-2 \end{cases} \\ e(v_{p-1}) &= e(v_i) + 1 = p-1-i \\ e(v_p) &= e(v_j) + 1 = j. \end{aligned}$$

Now

$$\begin{aligned} \sum_{k=1}^{p} e(v_k) &= \sum_{k=1}^{\lceil \frac{p-2}{2} \rceil} (p-2-k) + \sum_{k=\lceil \frac{p-2}{2} \rceil + 1}^{p-2} (k-1) + p - 1 - i + j \\ &= \zeta(P_{p-2}) + p + j - i - 1. \end{aligned}$$

By Theorem 1,

$$\begin{aligned} \zeta(P_p) &= \left\lfloor \frac{3p^2-2p}{4} \right\rfloor \\ &= \left\lfloor \frac{3(p-2)^2 - 2(p-2)}{4} \right\rfloor + p + j - i - 1 \\ &= \left\lfloor \frac{3p^2-14p}{4} \right\rfloor + p + j - i + 3. \end{aligned}$$

$\zeta(G)$ is maximum when i is minimum and j is maximum, and the maximum value is $B = \lfloor \frac{3p^2-14p}{4} \rfloor + p + (p-3) - 2 + 3 = \lfloor \frac{3p^2-14p}{4} \rfloor + 2p - 2$. $\zeta(G)$ is minimum when i is maximum and j is minimum, and the minimum value is $A = \lfloor \frac{3p^2-14p}{4} \rfloor + p + \lceil \frac{p-2}{2} \rceil + 1 - \lceil \frac{p-2}{2} \rceil + 3 = \lfloor \frac{3p^2-14p}{4} \rfloor + p + 4$. Thus, $[A, B] = \left[\lfloor \frac{3p^2-14p}{4} \rfloor + p + 4, \lfloor \frac{3p^2-14p}{4} \rfloor + 2p - 2\right]$ is a p-total eccentric interval. □

Remark 3 From Theorem 2, $[A_3, B_3] = \left[\left\lfloor \frac{3p^2-6p-17}{4}\right\rfloor, \left\lfloor \frac{3p^2-6p-9}{4}\right\rfloor\right]$. Since the length of the interval $[A, B]$ is $p-6$, the length of the interval $[A_3, B_3]$ is 2 and $B_3 = B$, $[A_3, B_3]$ is a subinterval of $[A, B]$ for $p \geqslant 8$. For $6 \leqslant p \leqslant 14$, $[A_4, B_4] \cap [A, B] = \varnothing$ and for $p \geqslant 15$, $[A_4, B_4] \cap [A, B] \neq \varnothing$. But $A - B_5 = 10$, for all $p \geqslant 6$. This implies that $[A_k, B_k] \cap [A, B] = \varnothing$ for $5 \leqslant k \leqslant p-2$. From these, it may be concluded that the p-total eccentric interval $[A, B]$ obtained in Theorem 5 is an extension of either $[A_3, B_3]$ or $[A_4, B_4]$ obtained in Theorem 2 and disjoint from $[A_k, B_k]$ for $5 \leqslant k \leqslant p-2$.

Theorem 6 *Let G be graph on $p \geqslant 3$ vertices with at least two full degree vertices and e be an edge of G then*

$$\zeta(G-e) = \begin{cases} \zeta(G) + 2 & \textit{if end vertices of e are full degree vertices,} \\ \zeta(G) + 1 & \textit{if exactly one end vertices of e is full degree vertex,} \\ \zeta(G) & \textit{if both end vertices of e are not full degree vertices.} \end{cases}$$

Proof: Let $v_1, v_2, \ldots, v_k$ be the full degree vertices and $v_{k+1}, \ldots, v_p$ be the remaining vertices of G and e be an edge of G.

Case(i): End vertices of e are full degree vertices. Let $e = v_i v_j$, $1 \leqslant i, j \leqslant k$ and $i \neq j$. In $G - e$,

$$e_{G-e}(v_l) = \begin{cases} e_G(v_l) + 1 & \text{if either } l = i \text{ or } l = j, \\ e_G(v_l) & \text{otherwise.} \end{cases}$$

and hence, the result follows.

Case(ii): Exactly one end vertex of e is a full degree vertex say v_i. In $G - e$,

$$e_{G-e}(v_l) = \begin{cases} e_G(v_l) & \text{if } l \neq i, \\ e_G(v_l) + 1 & \text{if } l = i. \end{cases}$$

Case(iii): End vertices of e is not a full degree vertices. Let $e = v_i v_j$, $k+1 \leqslant i, j \leqslant p$ and $i \neq j$. In $G - e$, $e_{G-e}(v_l) = e_G(v_l)$ for $1 \leqslant l \leqslant p$. Hence, the result follows. □

Theorem 7 *For any positive integer $k \geqslant 4$, $\left[(4k-2)2^k - k + 2 - 2^{k-1}, (4k-2)2^k - k + 2\right]$ is a p-total eccentric interval when $p = 2^{k+1} - 1$.*

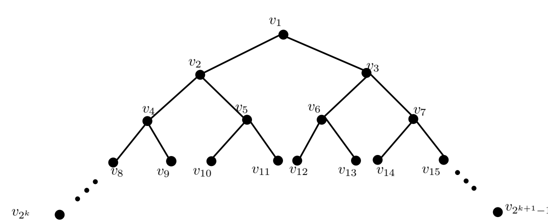

Fig. 2 Binary Tree with $v_{2^{k+1}-1}$ vertices.

Proof: Consider a binary tree T with $2^{k+1} - 1$ vertices for $k \geqslant 4$. T is labelled as shown in Fig. 2. The degree sequence of T is

$$d(v_i)=\begin{cases}2 & \text{for } i=1,\\ 3 & 2\leqslant i\leqslant 2^k-1,\\ 1 & 2^k\leqslant i\leqslant 2^{k+1}-1.\end{cases}$$

The eccentricity of the vertices of T are

$$e(v_i)=\begin{cases}k & \text{for } i=1,\\ k+j & 2^j\leqslant i\leqslant 2^{j+1}-1,\ j=1,2,\dots,k-1,\\ 2k & 2^k\leqslant i\leqslant 2^{k+1}-1.\end{cases}$$

Hence, the total eccentricity of T is

$$\begin{aligned}\zeta(T)&=\sum_{i=1}^{2^{k+1}-1} e(v_i)\\ &=e(v_1)+\sum_{i=2}^{2^k-1} e(v_i)+\sum_{i=2^k}^{2^{k+1}-1} e(v_i)\\ &=k+\sum_{j=1}^{k-1}\sum_{i=2^j}^{2^{j+1}-1}(k+j)+\sum_{i=2^k}^{2^{k+1}-1}2k\\ &=k+k(2+2^2+\cdots+2^{k-1})+(1(2)+2(2^2)\\ &\quad+\cdots+(k-1)(2^{k-1}))+(2k)2^k\\ &=(4k-2)2^k-k+2.\end{aligned}$$

Consider a path $v_i v_{\lfloor \frac{i}{2}\rfloor} v_{\lfloor \frac{i}{4}\rfloor} v_{\lfloor \frac{i}{8}\rfloor}$ for any $i=2^k$, 2^k+4, 2^k+8, $\dots$, $2^{k+1}-4$. For a fixed value of i, if we join v_i and $v_{\lfloor \frac{i}{4}\rfloor}$ by an edge, the total eccentric index of this new graph is $\zeta(T)-1$. Again, if we join v_i and $v_{\lfloor \frac{i}{8}\rfloor}$ by an edge, the total eccentric index of this new graph is $\zeta(T)-2$. Applying the above procedure to all i, the total eccentric index of the resultant graph is $\zeta(T)-2^{k-1}$. Hence, for any $k\geqslant 4$, $\left[(4k-2)2^k-k+2-2^{k-1},\ (4k-2)2^k-k+2\right]$ is a p-total eccentric interval when $p=2^{k+1}-1$. □

CONCLUSION

In this paper, we consider the inverse problem of the topological index for the total eccentric index. This study employs a novel method to address the question,"Is there a simple connected graph G of order p whose total eccentric index $n\in[\alpha,\beta]$?" as opposed to the conventional inverse problem. We studied such intervals and tried to extend their lengths by using different graph constructions. Also, find some free intervals for which no graph exists. These findings are useful for the construction of new molecular structures. These findings are also significant in determining the existence or non-existence of a particular molecular structure in the study of computer-aided drug designs and chemical graph theory.

Acknowledgements: The first author (Reg. No. 18147891155), is also a part-time research scholar at Anna University, Chennai, and wishes to express his sincere thanks to Mepco Schlenk Engineering College, Sivakasi, for fostering a culture of research and providing unwavering support in the academic and research journey.

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