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The eccentric connectivity index of $TUC_4C_8(R)$ nanotubes

A.R. Ashrafi[1], T. Došlić[2], M. Saheli[1]

[1]Department of Mathematics, Faculty of Science, University of Kashan, Kashan 87317-51167, I. R. Iran

[2]Faculty of Civil Engineering, University of Zagreb, Kačićeva 26, 10000 Zagreb, Croatia

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Abstract

The eccentric connectivity index $\xi(G)$ of a graph G is defined as $\xi(G) = \sum_{u\in V(G)} deg(u)\varepsilon(u)$, where $deg(u)$ denotes the degree of the vertex u and $\varepsilon(u)$ is the largest distance between u and any other vertex v of G. In this paper we present exact formulas for the eccentric connectivity index of $TUC_4C_8(R)$ nanotubes.

1 Introduction

All graphs considered in this paper are simple and connected. For two vertices u, v of a graph G their **distance** $d(u, v)$ is defined as the length of any shortest path connecting u and v in G. For a given vertex u of G its **eccentricity** $\varepsilon(u)$ is the largest distance between u and any other vertex v of G. The maximum eccentricity over all vertices of G is called the **diameter** of G and denoted by $D(G)$ and the minimum eccentricity among the vertices of G is called **radius** of G.

A **topological index** is a numerical quantity related to a graph that is invariant under graph automorphisms. Many topological indices have been defined and used in

QSAR/QSPR studies over the course of last decades. One of them is the **eccentric connectivity index** of a graph G. It is denoted by $\xi(G)$ and defined as

$$\xi(G) = \sum_{u \in V(G)} deg(u)\varepsilon(u).$$

This quantity has been recently used in several papers on structure-property and structure-activity relationships [1–5], and its mathematical properties have been investigated [6–9].

The eccentric connectivity index belongs to the family of distance-based topological indices. A group of researchers investigated recently a number of such indices and computed their values for a family of structures known as $TUC_4C_8(R)$ nanotubes and nanotori [10–21]. A $TUC_4C_8(R)$ nanotube is a mathematically beautiful object constructed from squares and octagons. An example is shown in Fig. 1. The aim of this paper is to compute the eccentric connectivity indices of such nanotubes.

Figure 1: Three-dimensional perception of a $TUC_4C_8(R)$ nanotube.

The terminology we use is standard and mainly taken from standard graph theory textbooks such as, e.g., [22]. We encourage the reader to consult [10-13,15,17] and the references therein for basic properties of the nanotubes of the type considered here.

Throughout this paper $T[p, q]$ denotes a $TUC_4C_8(R)$ nanotube parameterized by the number of octagons in a fixed row (p) and column (q) of a 2-dimensional lattice such as shown in Fig. 2. The nanotube is obtained from the lattice by wrapping it up so that each dangling edge from the left-hand side connects to the rightmost vertex

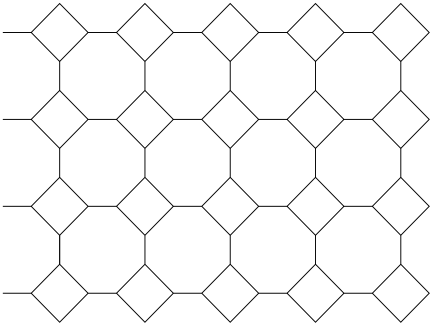

Figure 2: The 2-dimensional lattice of $T[4,3]$ nanotube.

of the same row. The reader should notice that the number of both squares and octagons in one layer of the nanotube is equal to $p+1$. As each vertex of $TUC_4C_8(R)$ is contained in exactly one square, the number of vertices of the nanotube is equal to $4(+1)(q+1)$. Similarly, the number of edges is given by $(p+1)(6q+5)$.

It is obvious that there is no loss of generality if we assume that the axis of the tube is vertical; hence it makes sense to use terms like top, bottom, above, below, etc. We label the rows of squares from top to bottom by labels $0, 1, \ldots, q$. It is also obvious from the symmetry of the nanotube that all squares in the same row are equivalent. Hence we need not bother to distinguish them or give them any labels. Vertices of a square in row i are denoted by v_i^+ (the top vertex), v_i^- (the bottom vertex) and v_i^0 (the remaining two vertices). If a need arises to distinguish between the two vertices denoted by v_i^0, we will denote them by v_{il}^0 and v_{ir}^0, where l and r stand for left and right, respectively. When the position of vertices in a square is not important, we use the wild-card convention v_i^*, where $*$ stands for any (or all) of $+$, $-$, or 0. The notation is exhibited in Fig. 3.

2 Main Results

Let us consider an arbitrary $TUC_4C_8(R)$ nanotube. Our first and most important task is to compute the eccentricities of the vertices in its top row. Once we know $\varepsilon(v_0^*)$ for given p and q, we can compute the eccentric connectivity index of an arbitrary nanotube of this type by summing the eccentricities of the vertices in

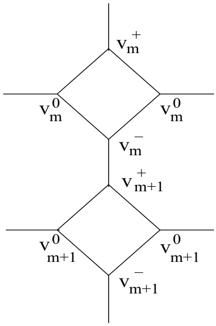

Figure 3: Notational conventions for vertices of a $T[p, q]$ nanotube.

rows q, $q-1, \ldots, \lfloor \frac{q+1}{2} \rfloor$ and doubling the result. (A correction might be needed for the equatorial row, depending on the parity of q.) We start by three auxiliary propositions.

Proposition 1
Any shortest path between v_0^* and v_m^* contains exactly one vertical edge of the form $v_i^- v_{i+1}^+$ for $i = 0, \ldots, m-1$, and no vertical edges below the level m. ■

Proposition 2
The eccentricity $\varepsilon(v_0^*)$ of a vertex v_0^* can be achieved only on a vertex from the bottom row. ■

Proposition 3
If the eccentricity of a vertex v_0^* is achieved on a vertex v_q^+, then it is also achieved on some other vertex of the same square.

Proof
Consider the situation shown in Fig. 4. Let $\varepsilon(v_0^*) = d(v_0^*, v_q^+)$. If $d(v_0^*, v_{ql}) > d(v_0^*, v_q^+)$ we have a contradiction. Hence $d(v_0^*, v_{ql}) \leq d(v_0^*, v_q^+)$. If the equality holds, we have the claim of the Proposition. Suppose, then, that $d(v_0^*, v_{ql}) < d(v_0^*, v_q^+)$. Then, necessary, $d(v_0^*, v_{ql}) = d(v_0^*, v_q^+) - 1$. Moreover, $d(v_0^*, v_{ql}) = d(v_0^*, v_{qr}) = d(v_0^*, v_q^+) - 1$. But then $d(v_0^*, v_q^-) = d(v_0^*, v_q^+) = \varepsilon(v_0^*)$, and we have the claim. ■

Hence the eccentricities of the vertices from the top row of squares are achieved on vertices from the lower border of the nanotube.

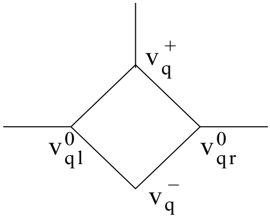

Figure 4: With proof of Lemma 3.

Now we make a digression and consider a closely related type of nanotubes that arise as Cartesian products of paths and cycles. Let $U[p,q] = C_{p+1} \Box P_{q+1}$ be one such nanotube. It is intuitively clear and it can be easily formalized that the diameter of such nanotube is achieved along a path from a vertex of the top row to a (diametrally opposite) vertex of the bottom row. Each such path has, roughly speaking, length of $\lfloor \frac{p}{2} \rfloor + q$. Each such path must have a certain number of turns or direction changes; this number must be at least one, and at most $2\min\{\lfloor \frac{p}{2} \rfloor, q\}$. We denote this quantity by r. The shortest paths with exactly r turns will be of special interest; two such paths are shown in Fig. 5. The computation of the eccentric connectivity indices

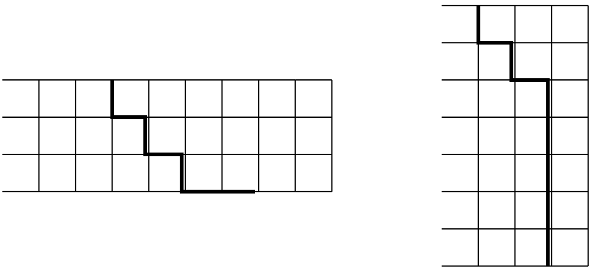

Figure 5: Shortest paths with maximum number of turns in a short (left) and in a long (right) nanotube.

of such nanotubes is now straightforward, and we refer the reader to [8] for more detail.

The nanotube of the above type are important in the present context since the $TUC_4C_8(R)$ nanotubes arise from $C_p \Box P_q$ nanotubes *via* truncation. (The truncation $Tr(G)$ of a given graph G is a graph obtained by replacing each vertex v of G by a $deg(v)$-gon aligned so that its vertices lie on the edges incident with v; the original vertices are then omitted. A truncation of simple graph with n vertices and m edges results in a cubic graph on $2m$ vertices and $3m$ edges. If all vertices in the original graph have degree at least 3, the resulting graph is also simple.) To be precise, in order to obtain $T[p,q]$ from $C_{p+1}\Box P_{q+1}$ one must truncate it and then subdivide by a vertex the edges in triangles on both borders. However, the effects of those edge subdivisions are of marginal importance for the following discussion.

Let us now look at what happens to a diametral path in $C_{p+1}\Box P_{q+1}$ after truncation. If the path passes trough a vertex v without changing direction, the number of steps increases by 2; if the path makes a turn in v, the number of steps increases by 1. (See Fig. 6.) Of all diametral paths in $C_{p+1}\Box P_{q+1}$ only those with maximum number

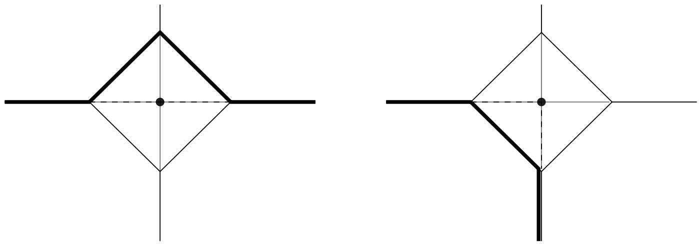

Figure 6: Truncation of a path passing straight through (left) and a path changing direction (right) in a vertex.

of turns will give rise to diametral paths in the truncated nanotube. Hence, the length of a diametral path (and also the eccentricity of a vertex from the top row) in $T[p,q]$ will be, roughly, $\lfloor \frac{p}{2} \rfloor + q + r + 2|\lfloor \frac{p}{2} \rfloor - q|$. If the tube is short with respect to its girth, then $r = 2\min\{\lfloor \frac{p}{2} \rfloor, q\} = 2q$, $|\lfloor \frac{p}{2} \rfloor - q| = \lfloor \frac{p}{2} \rfloor - q$ and the diameter is, roughly, $3\lfloor \frac{p}{2} \rfloor + q$. If the nanotube is long, then $r \sim p$, $|\lfloor \frac{p}{2} \rfloor - q| = q - \lfloor \frac{p}{2} \rfloor$ and the diameter is approximately $3q + \lfloor \frac{p}{2} \rfloor$. Hence, the eccentricity of a vertex from the top row of $T[p,q]$ is either of the form $3\lfloor \frac{p}{2} \rfloor + q$ or of the form $3q + \lfloor \frac{p}{2} \rfloor$. The dividing line between "short" and "long" nanotubes is at $q \sim \lfloor \frac{p}{2} \rfloor$, and indeed both expressions coincide there.

With some care the above heuristic reasoning can be made exact. This results in small additive corrections in the obtained formulas. The corrections depend on various combinations of parities of p and q. As an illustration, we work out in some detail the case of even p and odd q. The remaining cases follow along the same lines.

We consider first the case $q < p/2$. By starting at a vertex v_0^* of the top row, descending as quickly as possible, and then going along the bottom row as far as we can, we can ascertain ourselves that all vertices in the top row of squares have the

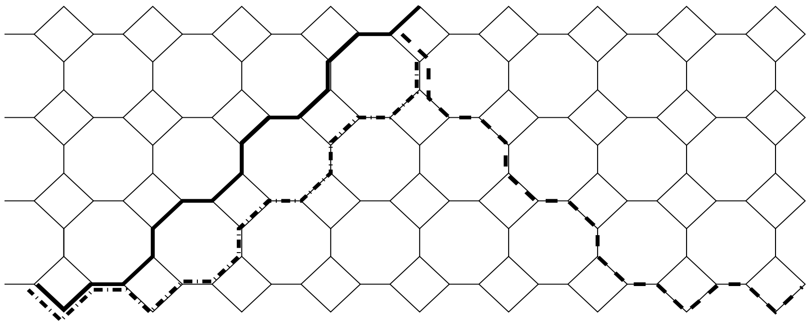

Figure 7: Extremal paths for the vertices of the uppermost row.

same eccentricity, $\varepsilon(v_0^*) = \frac{3}{2}p + q + 1$. The extremal paths starting in the vertices of the top row are shown in Fig. 7. Since row i is in no way different from row 0, we have $\varepsilon(v_i^*) = \frac{3}{2}p + q + 1$, for $i = 1, \ldots, \frac{q-1}{2}$. It remains to sum the contributions from all rows, taking into account the number of vertices in each row ($4(p+1)$) and their degrees. The last condition will force a separate treatment of the top row, since its v_0^+ vertices are of degree 2.

$$\begin{aligned}
\xi(T[p,q]) &= 2(p+1)\left[2\left(\frac{3}{2}p+q+1\right)+3\cdot 3\left(\frac{3}{2}p+q+1\right)\right.\\
&+ \left. 3\cdot 4\sum_{i=1}^{(q-1)/2}\left(\frac{3}{2}p+q+1-i\right)\right]\\
&= 2(p+1)\left[\frac{33}{2}p+11q+11+9pq+6q^2+6q-9p-6q-6-\frac{3}{2}q^2+\frac{3}{2}\right]\\
&= (p+1)[9q(2p+1)+15p+22q+13]
\end{aligned}$$

Next we consider the case $q \geq p$. Because of different parities of p and q it effectively means $q > p$, and hence $\frac{q-1}{2} \geq \frac{p}{2}$. Hence the vertices in all rows in the upper half of the nanotube will have the eccentricities of the form $3(q-i) + \frac{p}{2}$, with a possible additive correction. The correction can be determined by considering the shortest paths from the top row to the lower border, and it turns out to be dependent on the position of a vertex within the square. The dependence is very simple – the correction is equal to 2 for v_0^+, to 1 for v_0^0, and to 0 for v_0^-. Hence, $\varepsilon(v_0^+) = 3q+\frac{p}{2}+2$, $\varepsilon(v_0^0) = 3q + \frac{p}{2} + 1$ and $\varepsilon(v_0^-) = 3q + \frac{p}{2}$. Furthermore, $\varepsilon(v_i^*) = 3(q-i) + \frac{p}{2} + c$ for $i = 1, \ldots, \frac{q-1}{2}$, where $c = 2, 1$, or 0 for $* = +, 0, -$, respectively. The result for this case now follows by summing the contributions from all rows in the upper half of the nanotube (again treating the top row separately), and doubling the result of summation.

$$\begin{aligned}
\xi(T[p,q]) &= 2(p+1)\Big[2\left(3q+\frac{p}{2}+2\right)+6\left(3q+\frac{p}{2}+1\right)+3\left(3q+\frac{p}{2}\right)\\
&+ 3\sum_{i=1}^{(q-1)/2}\left(\left(3q+\frac{p}{2}+2-i\right)+\left(3q+\frac{p}{2}+1-i\right)+\left(3q+\frac{p}{2}-i\right)\right)\Big]\\
&= (p+1)[3q(9q+2p)+5+48q+17]
\end{aligned}$$

Finally we consider the most complicated case $\frac{p}{2} \le q < p$. The problem with this case is that the rows of the upper half of the nanotube belong to two different classes with respect to the formula for the eccentricity of their vertices. Those near the top will have the eccentricities of the form $3(q-i)+\frac{p}{2}$, those near the middle will have something like $\frac{3}{2}p+q-i$; in both cases some additive corrections may apply. The transition between two types occurs at row $\frac{p}{2}$, and it must be treated separately from the rest since the eccentricities of its vertices do not follow usual patterns. They are neither all equal, as in the case of $q < p/2$, nor all different, as in the case of $q > p/2$. Instead, we have $\varepsilon(v_{p/2}^+) = 2(p+1)$ and $\varepsilon(v_{p/2}^0) = \varepsilon(v_{p/2}^-) = 2p+1$. The result now follows by summing the contributions over all rows and multiplying the obtained sum by two.

$$\begin{aligned}
\xi(T[p,q]) &= 2(p+1)\Big[2\left(3q+\frac{p}{2}+2\right)+6\left(3q+\frac{p}{2}+1\right)+3\left(3q+\frac{p}{2}\right)\\
&+ 3\sum_{i=1}^{q-1-p/2}\left(\left(3q+\frac{p}{2}+2-3i\right)+\left(3q+\frac{p}{2}+1-3i\right)+\left(3q+\frac{p}{2}-3i\right)\right)\\
&+ 12\sum_{i=1}^{(p-q-1)/2}(2p+1-i)+6(p+1)+9(2p+1)\Big]\\
&= (p+1)(6p^2+33q^2-6pq+5p+42q+17)
\end{aligned}$$

The remaining parity combinations yield to the same type of analysis and we omit the details. Instead, we present the explicit formulas for $\xi(T[p,q])$ in a compact form valid for all combinations.

Theorem 4
The eccentric connectivity index of $T[p,q]$ is given by

$$\xi(T[p,q]) = \begin{cases} (p+1)[(9q^2+18pq+15p+22q+10)+R(p,q)] & q < \lfloor \frac{p}{} \rfloor \\ (p+1)[(6p^2-6pq+33q^2+5p+42q+14)+R(p,q)] & \lfloor \frac{p}{2} \rfloor \leq q < p \\ (p+1)[(27q^2+6pq+5p+42q+14)+R(p,q)] & q \geq p \end{cases}$$

Here $R(p,q) = \left[(6q+5)\frac{1-(-1)^p}{2} + 3\frac{1-(-1)^q}{2}\right]$. ■

By bringing the term $(p+1)$ inside the square brackets, the quantity $(p+1)R(p,q)$ can be interpreted in terms of numbers of edges and vertices of the nanotube as $\frac{1-(-1)^p}{2}|E(T[p,q])| + \frac{3}{4}\frac{1-(-1)^q}{2}|V(T[p,q])|$.

As a concluding remark, we point out that our method of reducing a $TUC_4C_8(R)$ nanotube to its $C_p \square P_q$ parent can be also successfully applied to all-hexagonal nanotubes. Apart from the results reported in [9] for hexagonal belts, we are not aware of any formulas for such nanotubes.

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