A NEW METHOD FOR COMPUTING DISTANCE-BASED TOPOLOGICAL INDICES OF $C_4C_8(R)$ NANOTUBES

MEHRDAD TAGHIZADEH, MAJID AREZOOMAND*, HAMID GAZOR
Department of Mathematics, Majlesi Branch, Islamic Azad University, Isfahan, Iran

In this work, a bijection between the vertices of the graph of $C_4C_8(R)$ nanotube and a subset of Z^4 is given. Then a distance function over this graph is defined. Using this distance function, all distance-based topological indices of the nanotube can be computed very easily. The diameter of the nanotube is computed as an example. Also a MATHEMATICA program is written for computing the distance-based topological indices of the nanotube.

(Received November 5, 2012; Accepted December 7, 2012)

Keywords: $C_4C_8(R)$ nanotube, Topological index, Diameter

1. Introduction

A topological index is a real number related to a graph of a molecule, which is structural. It does not depend on the labeling or pictorial representation of the graph. In recent years, there has been considerable interest in the general problem of determining topological indices of nanotubes and nanotori [1-6]. It has been established, for example, that Wiener and hyper-Wiener indices of polyhex nanotubes and tori are computable from the molecular graph of these structures. Accordingly, some of the interest has been focused on computing topological indices of these nanostructures. Let G be an undirected connected graph without loops or multiple edges, with vertex set $V(G)$ and the edge set $E(G)$. The distance between two vertices x and y is denoted by $d(x,y)$. The Wiener index $W(G)$ of G, which is the oldest topological index is a distance-based topological index and is defined as the sum of distances between all vertices of the graph:

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

There are some other distance-based topological indices. The hyper-Wiener index $WW(G)$ is defined as

$$WW(G)=\frac{1}{2}W(G)+\frac{1}{4}\sum_{\{u,v\}\subseteq V(G)} d(u,v)^2.$$

The diameter d of a graph is the largest distance between any two vertices, i.e. the largest $d(u,v)$ value in the distance matrix. Balaban and co-authors introduced the reverse Wiener index. They showed that starting from the distance matrix and subtracting from d each $d(u,v)$ value, one obtains a new symmetrical matrix which, like the distance matrix, has zeroes on the main diagonal and, in addition, at least one pair of zeroes of the main diagonal corresponding to the diameter in the distance matrix. The obtained general formula for reverse Wiener index of a graph G with N vertices and diameter is

$$\Lambda(G)=\frac{1}{2}N(N-1)d-W(G).$$

Let u and v be two adjacent vertices of the graph G and $e=uv$ be the edge between them. The Balaban index of a molecular graph is introduced by Balaban [7] as one of less degenerated

*Corresponding author: arezoomand@math.iut.ac.ir

topological indices. It calculates the average distance sum connectivity index according to the equation

$$J(G)=\frac{m}{\mu+1}\sum\nolimits_{uv\in E(G)}[d(u)d(v)]^{-0.5}$$

Where m is the number of edges in G and $\mu=m+n-1$ (n is the number of vertices of G) is the cyclomatic number of G and $d(u)=\sum\nolimits_{v\in V(G)}d(u,v)$ is the distance sum of a vertex u of G.

In this paper, a bijection between the vertices of $C_4C_8(R)$ nanotube and a subset of Z^4 is given. Then a distance function on the vertices of the graph is defined. Using this function, one can easily compute all distance-based topological indices of the graph. As examples some topological indices and the diameter of the graph are computed.

Theory and Results

Let $T=T[p,q]$ be the molecular graph of $C_4C_8(R)$ with p rhomb in every row and q rhomb in every column as shown in Figure 1.

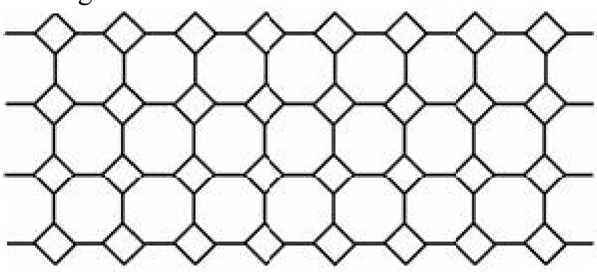

Fig.1. Two dimensional Lattice of T[8,4]

It is easy to see that T has $4pq$ vertices and $6pq-p$ edges. Consider the vectors

$$e_1=(1,0), e_2=(-\frac{\sqrt{2}}{2},-\frac{\sqrt{2}}{2}),\ e_3=(-\frac{\sqrt{2}}{2},\frac{\sqrt{2}}{2}),\ e_4=(0,1)$$

as shown in Figure 2. Put $a_1=e_1-e_2-e_3$ and $a_2=e_2-e_3-e_4$.

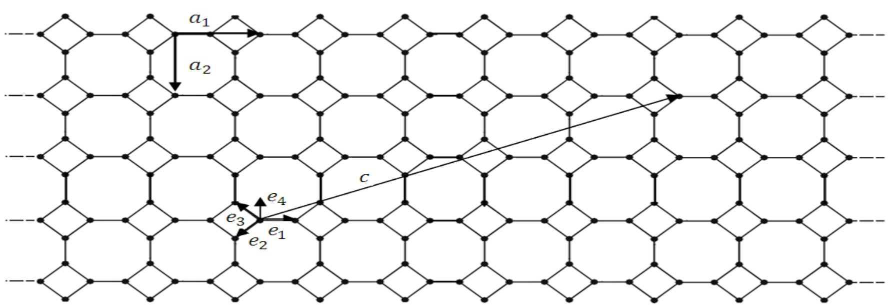

Fig.2. The vectors e_1, e_2, e_3 and e_4.

Now we give a mathematical model for $V(T)$, the vertices of T. Let a=(0,0,0,0), b=(0,1,0,0), c=(0,0,1,0) and d=(0,1,1,0). Then $V(T)=\{v+na_1+ma_2 \mid v=a,b,c,d,\ 0\leq n\leq p-1,\ 0\leq m\leq q-1\}$.

Theorem 1. Let $A=Z\cap[0,p-1]$ and $B=Z\cap[-q+1,0]$ where Z is the set of integers. There is a bijection

$$\phi:\ell\rightarrow V(T)$$

$$(x_1,x_2,x_3,x_4)\mapsto\sum_{i=1}^{4}x_ie_i$$

from the set $\ell = \{(x_1, x_2, x_3, x_4) \in Z^4 \mid x_1 \in A, x_2 \in B, x_1 + x_2 + x_4 \in \{0,1\}, x_1 + x_3 - x_4 \in \{0,1\}\}$ to the set of vertices of C_4C_8(R) nanotube $T=T[p,q]$.

Proof. By the geometry of *T*, it is clear that *Φ* is well-defined. We prove that this map is 1-1 and onto. Let $x=(x_1,x_2,x_3,x_4)$, $y=(y_1,y_2,y_3,y_4)$ and $\Phi(x)=\Phi(y)$. By considering the vectors e_i, $1 \le i \le 4$, and $\Phi(x)=\Phi(y)$, we have $y_1 - \frac{\sqrt{2}}{2}(y_2 + y_3) = y_1 - \frac{\sqrt{2}}{2}(y_2 + y_3)$ and $-\frac{\sqrt{2}}{2}(x_2 - x_3) + x_4 = -\frac{\sqrt{2}}{2}(y_2 - y_3) + y_4$. So

$$x_1 - y_1 = \frac{\sqrt{2}}{2}(x_2 + x_3 - (y_2 + y_3)) \ , \ x_4 - y_4 = \frac{\sqrt{2}}{2}(x_2 - x_3 - (y_2 - y_3)).$$

But the coordinates of *x* and *y* are integers, therefore $x_1=y_1$, $x_4=y_4$, $x_2+x_3=y_2+y_3$ and $x_2-x_3=y_2-y_3$. Consequently we have $x=y$. Therefore *Φ* is 1-1.

Now let $v \in V(T)$. Without loss of generality, let $v=b+na_1+ma_2$. Since $b=e_2$, $v=ne_1+(m-n+1)e_2-(m+n)e_3-me_4$, we have $\Phi(n,m-n+1,-m-n,-m)=v$ and it is easy to check that $(n,m-n+1,-m-n,-m)$ is an element of ℓ .■

It is easy to check that $\ell = \bigcup_{i=1}^{4} T_i$ where

$$T_1 = \{(x_1, x_2, x_3, x_4) \in \ell \mid x_1 + x_2 + x_4 = 0, x_1 + x_3 - x_4 = 0\},$$
$$T_2 = \{(x_1, x_2, x_3, x_4) \in \ell \mid x_1 + x_2 + x_4 = 0, x_1 + x_3 - x_4 = 1\},$$
$$T_3 = \{(x_1, x_2, x_3, x_4) \in \ell \mid x_1 + x_2 + x_4 = 1, x_1 + x_3 - x_4 = 0\},$$
$$T_4 = \{(x_1, x_2, x_3, x_4) \in \ell \mid x_1 + x_2 + x_4 = 1, x_1 + x_3 - x_4 = 1\}.$$

Lemma 1. Let $c=(p,-p,-p,0)$. For every two vertices $u=(u_1,u_2,u_3,u_4)$ and $v=(v_1,v_2,v_3,v_4)$ of T, we define

$$f(u,v) = \sum_{i=1}^{4} |u_i - v_i|$$

and

$$d(u,v) = Min\{f(u,v), f(u+c,v), f(u-c,v)\}.$$

Then $d(u,v)$ is the minimum distance between *u* and *v*.

Proof. It is clear that the chiral vector of *T* is $c=pa_1=pe_1-pe_2-pe_3=(p,-p,-p,0)$. Also after rolling up the lattice of T, every $u \in V(T)$ coincides with $u+c$ and $u-c$. But for every $x, y \in V(T)$, $f(x,y)$ is the minimum distance of *x* and *y* in the two dimensional lattice of the nanotube. So the result is clear.■

Corollary 1. Let $u=(u_1,u_2,u_3,u_4)$ and $v=(v_1,v_2,v_3,v_4)$ be two vertices of *T*. Then

$$d(u,v) = \begin{cases} f(u,v) & if \ |u_1 - v_1| < [p/2] \\ f(u+c,v) & if \ |u_1 - v_1| \ge [p/2], u_1 < v_1 \\ f(u-c,v) & f \ |u_1 - v_1| \ge [p/2], u_1 \ge v_1 \end{cases}.$$

Proof. From the geometry of T and the fact that the first coordinate of every corner of any rhomb in a fix row is fixed, the result is clear.■

Lemma 2. Let $u=(u_1,u_2,u_3,u_4)$, $v=(v_1,v_2,v_3,v_4)$, $u_1-v_1=r$ and $u_4-v_4=s$. Put $Max\{|r|,|s|\}=a$ and $Min\{|r|,|s|\}=b$. We have

$$f(u,v) = \begin{cases} 3a + b \pm (\varepsilon_2(u) - \varepsilon_2(v)) & if \ a = \pm s \\ 3a + b \pm (\varepsilon_1(v) - \varepsilon_1(u)) & if \ a = \pm r \end{cases}$$

where for any $x=(x_1,x_2,x_3,x_4)$,

$$\in_1(x)=\begin{cases}(-1)^{x_1+x_3-x_4} & if\ x\in T_1\cup T_4\\ 0 & otherwise\end{cases}$$
$$\in_2(x)=\begin{cases}(-1)^{x_1+x_3-x_4} & if\ x\in T_2\cup T_3\\ 0 & otherwise\end{cases}.$$

Proof. By definition of the function *f,* we have $f(u,v)=|r|+|s|+|u_2-v_2|+|u_3-v_3|$. From our model, it is clear that $|u_2-v_2|=s+r+g(u,v)$ and $|u_3-v_3|=s-r+h(u,v)$ where

$$g(u,v)=\begin{cases}0 & (u,v)\in T_i\times T_j,\ j=i\ or\ (i,j)=(1,2),(3,4)\\ 1 & (u,v)\in(T_3\cup T_4)\times(T_1\cup T_2)\\ -1 & (u,v)\in(T_1\cup T_2)\times(T_3\cup T_4)\end{cases},$$
$$h(u,v)=\begin{cases}0 & (u,v)\in T_i\times T_j,\ j=i\ or\ (i,j)=(1,3),(2,4)\\ 1 & (u,v)\in(T_2\cup T_4)\times(T_1\cup T_3)\\ -1 & (u,v)\in(T_1\cup T_3)\times(T_2\cup T_4)\end{cases}$$

Now we have $a\in\{r,-r,s,-s\}$. Without loss of generality, we assume that $a=r$. The proof of remaining cases are similar. In this case $r\geq 0$ and $|s|\leq r$. Let $s\neq\pm r$. Then $|u_2-u_3|+|v_2-v_3|=3r+|s|+g(u,v)-h(u,v)$. It is easy to check that $g(u,v)-h(u,v)=\varepsilon_1(v)-\varepsilon_1(u)$ and so in this case we get the result. Now let $s=r\neq 0$. Then $|u_2-u_3|+|v_2-v_3|=2r+g(u,v)+|h(u,v)|$ and so $f(u,v)=3r+|s|+g(u,v)+|h(u,v)|$.■

As an application of our mathematical model, we compute the diameter of T[p,q] nanotube.

Theorem 2. The diameter of T=T[p,q] is

$$d(T)=\begin{cases}p+q+[p/2]-1 & q<[(p+1)/2]\\ 3q+[p/2]-1 & q\geq[(p+1)/2]\end{cases}$$

Proof. From the geometry of T and its symmetry, it is clear that $d(T)=Max\{d((0,0,1,0),x)\mid x\in\ell\}$. Note that the vertex *(0,0,1,0)* is not unique with this property. It is easy to see that $d(T)=d((0,0,1,0),(x_1,x_2,x_3,x_4))$ if and only if $x_1=\frac{p}{2},x_4=-q+1$ when p is even, and $x_1=\frac{p-1}{2},x_4=-q+1$ when *p* is odd. But by Theorem 1, $x_2=-(x_1+x_4)$ or $x_2=-(x_1+x_4)+1$ and $x_3=x_4-x_1$ or $x_3=x_4-x_1+1$. So we must consider four cases. By similarity of computations we just consider the case that *p* is even and $q\leq[(p+1)/2]$.

In this case $x_1=p/2$ and $x_4=-q+1$ and $q\leq p/2$. So $x_2=-(p/2-q+1)$ or $-(p/2-q+1)+1$ and $x_3=-q-p/2+1$ or $-q-p/2+2$. If $x_2=-(p/2-q+1)$ and $x_3=-q-p/2+1$, then

$$d((0,0,1,0),(x_1,x_2,x_3,x_4))=f((0,0,1,0),(x_1-p,x_2+p,x_3+p,x_4))=p+q+p/2-2$$

If $x_2=-(p/2-q+1)+1$ and $x_3=-q-p/2+2$, then

$$d((0,0,1,0),(x_1,x_2,x_3,x_4))=f((0,0,1,0),(x_1-p,x_2+p,x_3+p,x_4))=p+q+p/2-2$$

In other subcases, we have $d((0,0,1,0),(x_1,x_2,x_3,x_4))=p+q+p/2-1$. Hence in this case the result is true.■

MATHEMATICA program for computing distance-based topological indices

Using our mathematical model and our distance function, we write some programs for computing distance-based topological indices of the nanotube as follows. Let A be the adjacency matrix and DD be the distance matrix of the graph of nanotube.

```
p=4:q=6: (for example)
a={0,0,0,0};b={0,1,0,0};c={0,0,1,0};d={0,1,1,0};
```

```
x={1,-1,-1,0};y={0,1,-1,-1};z={p,-p,-p,0};
V={};
For[i=0,i≤p-1,
   For[j=0,j≤q-1,
      AppendTo[V,a+i*x+j*y];
      AppendTo[V,b+i*x+j*y];
      AppendTo[V,c+i*x+j*y];
      AppendTo[V,d+i*x+j*y];
    j++];
i++];
ff[u_,v_]:=Sum[Abs[u[[i]]-v[[i]],{i,1,4}];
f[u_,v_]:=Min[ff[u,v],ff[u+z,v],ff[u-z,v]];
A=Table[t[i,j],{i,1,4p*q},{j,1,4p*q}];
 For[i=1, i≤4p*q,
     For[j=1, ,j≤4p*q,
         If[f[V[[i]],V[[j]]]==1,t[i,j]=1, t[i,j]=0];
     j++];
i++];
DD=Table[f[V[[i]],V[[j]]],{i,1,4p*q},{j,1,4p*q}];
MatrixForm[A];
MatrixForm[DD];
```

The outputs of the above program are the adjacency matrix A and the distance matrix DD.
By adding the line "W=0.5*Sum[Sum[DD[[i]][[j]],{i,1,4p*q}],{j,1,4p*q}]" one can compute the Wiener index of the graph. Also by adding
"WW=0.5*W+0.125*Sum[Sum[DD[[i]][[j]]^2, {i,1,4p*q}],{j,1,4p*q}]
one can obtain the hyper-Wiener index of the graph.
Also by adding the line
RW=2p*q*(4p*q-1)*Max[DD]-0.5*Sum[Sum[DD[[i]][[j]],{i,1,4p*q}],{j,1,4p*q}]
we get the reverse-Wiener index of the nanotube.

Acknowledgement

This research is supported by Islamic Azad University in Majlesi Branch (Grant No. 321).

References

[1] S. Yousefi, A.R. Ashrafi, An exact expression for the Wiener index of a polyhex nanotorus, MATCH Commun. Math. Comput. Chem. **56**, 169 (2006)
[2] M. Eliasi and B. Taeri, Balaban Index of zigzag polyhex nanotorus, J. Comput. Theor. Nanosci. **4**, 1174 (2007).
[3] A. Heydari, B. Taeri, Wiener and Schultz indices of $TUC_4C_8(S)$ nanotubes, MATCH Commun. Math. Comput. Chem. **57**, 665 (2007).
[4] M. Eliasi and B. Taeri, Distance in Zigzag polyhex nanotorus, J. Comput. Theor. Nanosci. **5**, 1029 (2008).
[5] A. Mahmiani, A. Iranmanesh and Y. Pakravesh, Szeged index of armchair polyhex nanotube, Ars Comb. **89**, 309 (2008).
[6] A. Iranmanesh and A. R. Ashrafi, Balaban index of an armchair polyhex, $TUC_4C_8(R)$ and $TUC_4C_8(S)$ nanotorus, J. Comput. Theor. Nanosci. **4**, 514 (2007) .
[7] A. T. Balaban, Highly discrimiting distance-based topological index, Chem. Phys. Lett. **80**, 399 (1982).