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TOPOLOGICAL INDICES OF SOME GRAPH PRODUCTS

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Abstract

A topological index is a numeric value derived from the structural graph of a molecule. Role of topological indices in chemistry began in 1947 when chemist Harold Wiener developed the most widely known topological descriptor, the Wiener index. In this paper, Wiener Polarity index, Harary Index, Estrada Index, Harary Estrada index, First Zagreb index of some graph products (Strong, Tensor) of P_m and P_n, P_m and C_n, C_m and C_n through Adjacency matrix are given.

I. Introduction

Our notation is standard and taken from the standard book of Graph theory [1]. Consider G is simple, connected graph with vertex set V and edge set E. If G is a molecular graph with n vertices, then its adjacency matrix A_{ij} is a square matrix of order n defined as $a_{ij} = 1$, if there is an edge between i^{th} and j^{th} vertices, $a_{ij} = 0$, if there is no edge between them. The Wiener index $W(G)$ of a connected graph G is defined as the sum of the distances between all pairs (ordered) of vertices of G [22]. Another important molecular descriptor was also introduced by Wiener [22], called the Wiener polarity index $Wp(G)$. It is defined as the number of unordered pairs of vertices that are at distance 3 in G. The Harary index is introduced by Plavsic et al., [7, 16]. It defined as the sum of reciprocals of distances between all pairs of vertices of a connected graph. Energy of the molecular graph G is defined by

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$E(G) = \sum_{i=1}^{n} | \lambda_i |$, where $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigen values of G. The Estrada index is defined as $EE(G) = \sum_{i=1}^{n} e^{\lambda_i}$, where $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigen values of G [8]. Harary matrix of a graph G is defined as a square matrix $H = H(G) = \left[\frac{1}{d(i, j)}\right]$, where $d(i, j)$ is the distance between the vertices v_i and v_j in G. The eigenvalues of the Harary matrix $H(G)$ are denoted by $\rho_1, \rho_2, \ldots, \rho_n$ and are said to be the H-eigenvalues of G. Harary Energy of the molecular graph G is defined by $E(G) = \sum_{v \in G}^{n} | \rho_i |$, where $\rho_1, \rho_2, \ldots, \rho_n$ be the H-eigen values of G. Harary Estrada index of G, denoted by $HEE(G)$, where $HEE(G) = \sum_{v \in G}^{n} e^{\rho_i}$, where $\rho_1, \rho_2, \ldots, \rho_n$, be the H-eigen values of G [2]. The first Zagreb index of G is defined as $M_1 = \sum_{v \in G} d(v)^2$ [3, 4]. Wiener index of any graph through adjacency matrix using MATAB given in [19]. And also Wiener index of Harary graph through adjacency matrix using MATAB given in [18]. In particular, Wiener index of graph product and some nanostructures calculated through adjacency matrix using MATLAB given in [20, 21]. In this paper, to overcome time complexity MATLAB program is used for finding some topological indices through adjacency matrix of two standard graph products (Tensor, Strong) of path and path, path and cycle, cycle and cycle. In [5, 6], Imrich and Izbickihave discussed about the product graphs in detail. The symbols used to denote products are based mainly on those found in [5, 6, 10]. The above topological indices of the product graphs was much studied in [5, 6, 17].

II. Graph Product

Definition 2.1 Strong Product [12, 15]**.** Strong product $G \boxtimes H$ of graphs G and H is a graph such that the vertex set of $G \boxtimes H$ is the Cartesian product $V(G) \times V(H)$ and any two distinct vertices (u, u') and (v, v') are adjacent in $G \boxtimes H$ if and only if u is adjacent to v and $u' = v'$, or $u = v$ and u' is adjacent to v', or u is adjacent to v and u' is adjacent to v'. The strong product is also called the normal product and product.

Definition 2.2. Tensor Product [9, 11]**.** Tensor product $G \times H$ of graphs G and H is a graph such that the vertex set of $G \times H$ is the Cartesian product $V(G) \times V(H)$ and any two vertices (u, u') and (v, v') are adjacent in $G \times H$ if and only if u' is adjacent with v' and u is adjacent with v. The tensor product is also called as the direct product, categorical product, cardinal product, relational product, Kronecker product, weak direct product, or conjunction.

An Algorithm for Computing the Topological Index of Some Product Graphs

Let G, H be two connected graphs, whose vertex set are V_1 and V_2 respectively, where $|V_1| = m, |V_2| = n.$ then the product of G and H has mn vertices. In this section, we present an algorithm for obtaining some topological indices of $P_m \boxtimes P_n$, $P_m \boxtimes C_n$, $C_m \boxtimes C_n$, $P_m \times P_n$, $P_m \times C_n$, $C_m \times C_n$

1. Input number of vertices of G and number of vertices of H

2. Label the vertices of the product graph by the set of natural numbers $\{1, 2, \ldots, mn\}$ in some manner (*)

3. Frame the Generalized Adjacency matrix of the given product graph.

*-For Strong product of two graphs G and H, label the vertices as $1, 2, \ldots, m$ in the First row and the vertices $m+1, \ldots, 2m$ in the second row. In the similar manner, vertices $(n-1)m+1 \ldots mn$ in the nth row. (refer Figure 1).

III. Strong Product

In this Section, the program is given for finding adjacency matrix of Strong product of P_m and P_n, P_m and C_n, C_m and C_n for arbitrary $m, n.$ Since this product is commutative.

3.1. Strong Product of P_m and P_n

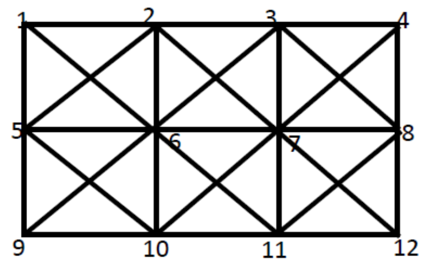


Figure 1. $P_4 \boxtimes P_3$.

% Program to calculate the adjacency matrix of $P_m \boxtimes P_n$

```
m= input('Path with vertices m=');
n= input('Path with vertices n=');
A=[];
for i=1:(n*m)-m
A(i,i+m)=1;A(i+m,i)=1;
end
while i<=(m*n)-1
for i=1:(m*n)-1
A(i,i+1)=1;A(i+1,i)=1;
if rem(i,m)==0
A(i,i+1)=0;A(i+1,i)=0;
end
end
i=i+1;
end
for i=1:n*m
while i<=(n*m)-m-1
A(i,i+m+1)=1;A(i+m+1,i)=1;
```

```
if rem(i,m)==0
A(i,i+m+1)=0;A(i+m+1,i)=0;
end
    i=i+1;
end
end
for i=1:n*m
while i<=(n*m)-m
A(i+1,i+m)=1;A(i+m,i+1)=1;
if rem(i,m)==0&&m==2
A(i+1,i+m)=1;A(i+m,i+1)=1;
elseif rem(i,m)==0&&m>2
A(i+1,i+m)=0;A(i+m,i+1)=0;
end
    i=i+1;
end
end
A;
```

3.2. Strong Product of P_m and C_n

% Program to calculate the adjacency matrix of $P_m \boxtimes C_n$

```
m= input('Path with vertices m=');
n= input('Cycle with vertices n=');
A=[];
for i=1:(n*m)-m
A(i,i+m)=1;A(i+m,i)=1;
```

```
end
while i<=(m*n)-1
for i=1:(m*n)-1
A(i,i+1)=1;A(i+1,i)=1;
if rem(i,m)==0
A(i,i+1)=0;A(i+1,i)=0;
end
end
i=i+1;
end
for i=1:n*m
while i<=(n*m)-m-1
A(i,i+m+1)=1;A(i+m+1,i)=1;
if rem(i,m)==0
A(i,i+m+1)=0;A(i+m+1,i)=0;
end
    i=i+1;
end
end
for i=1:n*m
while i<=(n*m)-m
A(i+1,i+m)=1;A(i+m,i+1)=1;
if rem(i,m)==0&&m==2
A(i+1,i+m)=1;A(i+m,i+1)=1;
elseif rem(i,m)==0&&m>2
A(i+1,i+m)=0;A(i+m,i+1)=0;
```

```
end
    i=i+1;
end
end
for i=1:m
A(i,i+(m*(n-1)))=1;A(i+(m*(n-1)),i)=1;
end
for i=1:m-1
    A(i,i+(m*(n-1))+1)=1;A(i+(m*(n-1))+1,i)=1;
end
for i= 1:m-1
A(i+1,i+(m*(n-1)))=1;A(i+(m*(n-1)),i+1)=1;
end
A;
```

3.3. Strong Product of C_m and C_n

% Program to calculate the adjacency matrix of $C_m \boxtimes C_n$

```
m= input('Cycle with vertices m=');
n= input('Cycle with vertices n=');
A=[];
for i=1:(n*m)-m
A(i,i+m)=1;A(i+m,i)=1;
end
while i<=(m*n)-1
for i=1:(m*n)-1
A(i,i+1)=1;A(i+1,i)=1;
```

```
if rem(i,m)==0
A(i,i+1)=0;A(i+1,i)=0;
end
end
i=i+1;
end
for i=1:n*m
while i<=(n*m)-m-1
A(i,i+m+1)=1;A(i+m+1,i)=1;
if rem(i,m)==0
A(i,i+m+1)=0;A(i+m+1,i)=0;
end
    i=i+1;
end
end
for i=1:n*m
while i<=(n*m)-m
A(i+1,i+m)=1;A(i+m,i+1)=1;
if rem(i,m)==0&&m==2
A(i+1,i+m)=1;A(i+m,i+1)=1;
elseif rem(i,m)==0&&m>2
A(i+1,i+m)=0;A(i+m,i+1)=0;
end
    i=i+1;
end
end
```

```
for i=1:m
A(i,i+(m*(n-1)))=1;A(i+(m*(n-1)),i)=1;
A(1,(m*n))=1;A((m*n),1)=1;
A((m*n)-m+1,m)=1;A(m,(m*n)-m+1)=1;
end
for i=1:m-1
    A(i,i+(m*(n-1))+1)=1;A(i+(m*(n-1))+1,i)=1;
end
for i= 1:m-1
A(i+1,i+(m*(n-1)))=1;A(i+(m*(n-1)),i+1)=1;
end
for i=1:m:(m*n)-m+1
A(i,i+m-1)=1;A(i+m-1,i)=1;
end
for i=1:m:(m*(n-2)+1)
A(i,i+(2*m-1))=1;A(i+(2*m-1),i)=1;
end
for i=m:m:(m*n-m)
A(i,i+1)=1;A(i+1,i)=1;
end
A;
```

IV. Tensor Product

4.1. Tensor Product of P_m and P_n

Tensor Product of P_m and P_n is disconnected. Since $G \times H$ is connected if and only if both G and H are connected and at least one of them is non-bipartite. Furthermore, if both G and H are connected and bipartite, then

$G \times H$ has exactly two connected components. [11]

4.2. Tensor Product of P_m and C_n [14]

The following program illustrate Adjacency matrix of Tensor Product of P_m and C_n when m and n are odd or m is even and n is odd.

```
% Program to calculate the adjacency matrix of Pm × Cn

m= input('Path with vertices m=');

n= input('Cycle with vertices n=');

A=[];

for i=1:m-1

A(i,i+1)=1;A(i+1,i)=1;

end

B=[];

for j=1:n-1

B(j,j+1)=1;B(j+1,j)=1;

B(1,n)=1;B(n,1)=1;

end

C = kron(A,B);
```

4.3. Tensor Product of C_m and C_n [13]

The following program illustrate Adjacency matrix of Tensor Product of P_m and C_n when m and n are odd, m is even and n is odd, m is odd and n is odd. Since, Tensor Product of C_m and C_n is disconnected, when m and n are even

```
% Program to calculate the adjacency matrix of Cm × Cn

m= input('Cycle with vertices m=');

n= input('Cycle with vertices n=');

A=[];
```

```
for i=1:m-1
A(i,i+1)=1;A(i+1,i)=1;
A(1,m)=1;A(m,1)=1;
end
B=[];
for j=1:n-1
B(j,j+1)=1;B(j+1,j)=1;
B(1,n)=1;B(n,1)=1;
end
C = kron(A,B);
```

V. Illustration

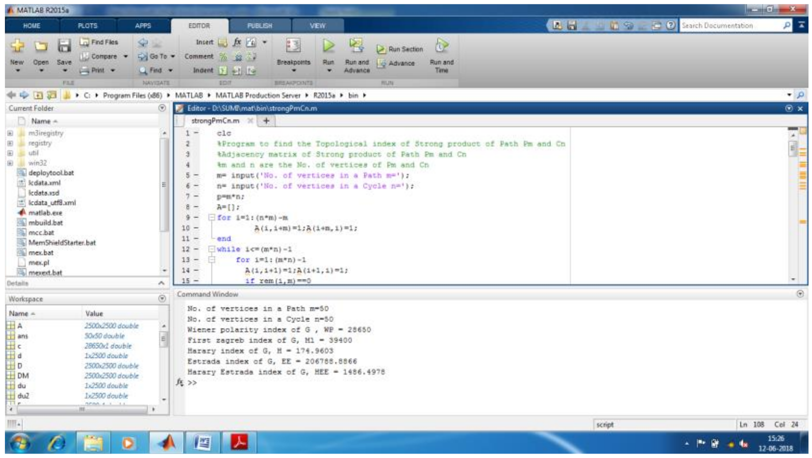
The following table represents Topological indices of standard graph product for arbitrary m, n.

Table 1. Topological indices of graph Products.

S.No.	Graph Product	m	n	Wiener polarity index	Harary index	Estrada index	Harary Estrada index	First Zagreb index
1.	$P_m \boxtimes P_n$	31	42	13707	191.1717	100394.9546	24524.8789	19964
2.	$P_m \boxtimes C_n$	50	50	28650	174.9603	206788.8866	1486.4978	39400
3.	$C_m \boxtimes C_n$	27	29	9396	101.5841	67312.3819	1328.7815	12528
4.	$P_m \times C_n$	45	25	6400	38.7901	101.0987	49.4216	176
5.	$C_m \times C_n$	20	15	1800	19.4464	45.5917	27.2177	80

VI. Execution of the Program

The following is the execution of Strong product of P_{50} and C_{50} in the command window



VII. Conclusion

According to MATLAB program, the topological indices of the standard products of well-known graphs can be computed quickly. The MATLAB program is tested to calculate the above topological indices of two standard products for arbitrary m, n.

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