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Spectral properties of some matrices related to topological indices

SAMANEH ZANGI[•]

Department of Mathematics, Faculty of Science, Shahid Rajaee

Teacher Training University, Tehran, 16785 – 136, I R. Iran

ABSTRACT. A topological index is a kind of molecular descriptor which anticipates some properties of chemical compound. The aim of this paper is to compute the spectrum of PA adjacency matrix associated to a well-known topological index.

Keywords: spectrum of graph, topological index, adjacency matrix.

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1. INTRODUCTION

Here, we introduce some basic notation and terminology used throughout the paper. All graphs considered here are finite and simple. A simple graph X is a graph without loops and multiple edges. The vertex set and the edge set of graph X are denoted by V(X) and E(X), respectively. When two vertices u and v are endpoints of an edge, we say that they are adjacent and write $u \sim v$ to indicate this. The adjacency matrix A is an $n \times n$ matrix whose xy-th entry is 1 if $xy \in E$ and zero otherwise.

The spectrum of a graph is based on the adjacency matrix of graph and it is strongly dependent on the form of this matrix. A number of possible disadvantages can be derived by using only the spectrum of a graph. For example, some information about expansion and randomness of a graph can be derived from the second largest eigenvalue of a graph. One of the main applications of graph spectra in chemistry is

[•]Author to whom correspondence should be addressed (E-mail: samanehzangi63@mail.com).

the application in Hückel molecular orbital theory for the determination of energies of molecular orbitals of π-electrons.

The real number λ is called the eigenvalue of graph Γ with adjacency matrix A if the equation $Ax = \lambda x$ has a nontrivial solution x. Then x is called eigenvector corresponding to the eigenvalue λ. The characteristic polynomial of the matrix A is $\chi_\lambda(G) = det(A - \lambda I)$ where the eigenvalues of A are roots of $\chi_\lambda(G)$.

2. MAIN RESULTS

For given graph G, if the maximum degree of every vertex reaches to four, then G is called a molecular graph. A topological index is a kind of molecular descriptor which anticipates some properties of chemical compound. Many topological indices were defined and many properties are discovered, see [1,2]. The first **inverse sum indeg index** (ISI index) defined as follows [3]:

$$ISI(G) = \sum_{uv \in E(G)} \frac{d_u d_v}{d_u + d_v}.$$

Let V(G)= {v_1,v_2,...,v_n} be the vertex set of graph G. For 1, 2, ...,n, let d_i be the degree of the vertex v_i. Then define the ISI adjacency matrix PA to be [4]

$$PA(G) = \begin{cases} \dfrac{d_i d_j}{d_i + d_j} & v_i \sim v_j \\ 0 & o.w \end{cases}.$$

If the graph G is regular of degree r, then $PA(G) = \frac{r}{2} A(G)$ and

$$PA^2(G) = \frac{1}{4} r^2 A^2(G). \tag{1}$$

Example 1. Let G be an r-regular graph. Since $tr\left(A^2\right) = 2m$, we have $tr(A^2(G)) = nr$. This means that $tr(PA^2(G)) = nr^3/4$.

Example 2. By using $Eq.$(1), we have $tr(PA^2(S_n)) = 2(n-1)^3/n^2$. Let P_n denotes to the path graph, then

$$PA(P_n) = \begin{bmatrix} 0 & 2/3 & & & & & \\ 2/3 & 0 & 1 & & & 0 & \\ & 1 & 0 & \ddots & & & \\ & & \ddots & 0 & 1 & & \\ & & & 1 & 0 & 2/3 \\ & 0 & & & 2/3 & 0 \end{bmatrix}.$$

The diagonal elements of PA^2 are $\frac{4}{9}, \frac{13}{9}, 2, 2, \ldots, 2, \frac{13}{9}, \frac{4}{9}$. Therefore

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$$tr(PA^2(P_n)) = \frac{34}{9} + 2(n-4) = 2n - \frac{38}{9}$$

Lemma 4. Let $PA(G) = \frac{r}{2}A(G)$, then

$$\chi_\lambda(PA(G)) = (\frac{r}{2})^n \chi_{\frac{2}{r}\lambda}(A(G)). \quad (2)$$

Proof. It is straightforward. For an example, $PA(S_n) = \frac{n-1}{n}A(S_n)$ and by using Lemma4 $\chi_\lambda(PA(S_n)) = (\frac{n-1}{n})^n \chi_{\frac{n\lambda}{n-1}}(A(S_n))$.

It is not difficult to see that $PA(K_{m,n}) = \frac{mn}{m+n}A(K_{m,n})$ and hence

$$\chi_\lambda(PA(K_{m,n})) = (\frac{mn}{m+n})^n \chi_{\frac{(m+n)\lambda}{mn}}(A(K_{m,n})) \quad (3)$$

Theorem 5 [4]. Let *G* be a graph with vertices set $\{1,2,\ldots,n\}$ and *ISI* matrix PA. Then

i) $tr(\mathrm{PA}) = 0, \quad (4)$

ii) $$tr(\mathrm{PA}^2) = 2\sum_{i\sim j}(\frac{d_id_j}{d_i+d_j})^2,\ (\mathrm{PA}^2)_{ij} = d_id_j\sum_{k\sim i,k\sim j}\frac{d_k^{\,2}}{(d_i+d_k)(d_j+d_k)}, \quad (5)$$

iii) $$tr(\mathrm{PA}^3) = 2\sum_{i\sim j}\frac{(d_id_j)^2}{d_i+d_j}(\sum_{k\sim i,k\sim j}\frac{(d_k)^2}{(d_i+d_k)(d_j+d_k)}), \quad (6)$$

iv) $$tr(\mathrm{PA}^4) = \sum_{i=1}^{n}(\sum_{i\sim l}(\frac{d_id_l}{d_i+d_l})^2)^2 + \sum_{i\neq j}d_id_j(\sum_{l\sim i,l\sim j}\frac{(d_l)^2}{(d_i+d_l)(d_j+d_l)})^2. \quad (7)$$

The probabilistic neural network PNN(*n, k, m*) can be constructed as follows:

There are three types of vertices in PNN(*n, k, m*), namely of degree *km*, of degree *n* + 1, and of degree *m*. Thus, we have $V_1 = \{v \in V(\mathrm{PNN}(n,k,m)) | d_v = km\}$, $V_2 = \{v \in V(\mathrm{PNN}(n,k,m)) | d_v = n+1\}$, and $V_3 = \{v \in V(\mathrm{PNN}(n,k,m)) | d_v = m\}$, where $|V_1| = n$, $|V_2| = km$ and $|V_3| = k$. Consequently, $|V(\mathrm{PNN}(n,k,m))| = v = |V_1|+|V_2|+|V_3| = n+k(m+1)$. There are two types of edges with respect to degrees of end vertices in PNN(*n, k,m*), namely with degrees of end vertices $\{km, n+1\}$ and degrees of end vertices $\{n+1, m\}$. Thus, we have

$$E_1 = E_{\{km,n+1\}} = \{uv \in E(\mathrm{PNN}(n,k,m)) | d_u = km, d_v = n+1\},$$

and

$E_2 = E_{\{n+1,m\}} = \{uv \in E(\mathrm{PNN}(n, k,m))|d_u = n + 1, d_v = m\}$, where $|E_{\{km,n+1\}}| = kmn$ and $|E_{\{n+1,m\}}| = km$. Consequently, $|E(PNN(n, k,m))| = e = |E_1| + |E_2| = km(n + 1)$. The probabilistic neural network $PNN(4, 2, 3)$ is depicted in Figure 1.

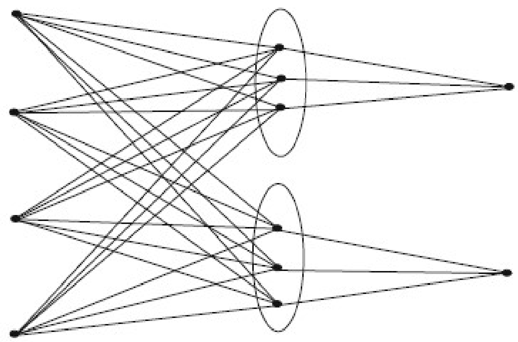

Figure 1. probabilistic neural network PNN(4, 2, 3).

The aim of this paper is to compute the spectrum of PA matrix of probabilistic neural network $PNN(n, k, m)$.

Theorem A. The spectrum of PA matrix of $PNN(n, k,m)$is as follows:

$$.\left\{[0]^{km+n-k},[\pm a\sqrt{m}]^{k-1},[\pm\sqrt{ma^2+kmb^2n}]^1\right\}.$$

Proof. One can easily prove that the PA matrix is as follows:

$$PA=\begin{bmatrix} 0_{k\times k} & C_{k\times mk} & 0_{k\times n} \\ C^t_{mk\times k} & 0_{mk\times mk} & D_{mk\times n} \\ 0_{n\times k} & D^t_{n\times mk} & 0_{n\times n}\end{bmatrix}$$

where

$$C=\begin{bmatrix} a & \cdots & a & 0 & 0 & \cdots & \cdots & \cdots & 0 \\ 0 & \cdots & 0 & a & \cdots & a & 0 & \cdots & 0 \\ \vdots & & & & & & & & \vdots \\ \vdots & & & & & & & & \vdots \\ 0 & 0 & \cdots & \cdots & \cdots & 0 & a & \cdots & a \end{bmatrix}$$

and

$$D = bJ\ ,\ b = \frac{mk(n+1)}{mk+n+1},\ a = \frac{m(n+1)}{m+n+1}.$$

This yields that if $\det(\mathrm{P}A - \lambda I) = 0$ then and so

$$\chi(PNN(n,\ k,m),\lambda) = (ma^2 - \lambda^2)^{k-1} \times \lambda^{km+n-k} \times (-kmb^2n - ma^2 + \lambda^2).$$

Hence,

$$\begin{vmatrix} xI_k & 0 & 0 \\ 0 & M & 0 \\ \frac{mba}{\lambda}J & P & S \end{vmatrix} = 0,$$

where

$$S = \begin{bmatrix} -\lambda & 0 & 0 & 0 \\ 0 & \ddots & \ddots & 0 \\ 0 & 0 & -\lambda & 0 \\ \lambda & \cdots & \lambda & y \end{bmatrix}_{n\times n},\ y = -\frac{kmb^2n}{x} - \lambda.$$

This means that

$$Spec(PA) = \begin{pmatrix} 0 & a\sqrt{m} & -a\sqrt{m} & \sqrt{ma^2 + kmb^2n} & -\sqrt{ma^2 + kmb^2n} \\ km+n-k & k-1 & k-1 & 1 & 1 \end{pmatrix}.$$

CONCUSION

In the studies of quantitative structure-activity relationship and quantitative structure-property relationship, the topological indices are utilized to guess the physical features related to the bioactivities and chemical reactivities in certain networks.

In this paper, we first defined a new matrix associated to the ISI index and then we computed it for several well-known graphs. In continuing of this paper, we computed its spectrum for probabilistic neural network *PNN*(*n, k, m*).

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