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On the Eigenvalues of some Matrices Based on Vertex Degree

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ABSTRACT

The aim of this paper is to first compute some bounds for forgotten index and then to present spectral properties of this topological index. In continuing, we define a new version of energy namely ISI energy corresponding to the ISI index. Finally, we determine some bounds for this new graph invariant.

1. INTRODUCTION

All graphs considered in this paper are connected, undirected and finite without loops and multiple edges. Denoted by $V(G)$ and $E(G)$, we mean the set of vertices and the set of edges of graph G, respectively.

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. Furtula and Gutman[2] introduced the forgotten index which is a special case of **general first Zagreb index** and studied its basic properties. In this paper some application of forgotten index in chemistry is also presented and the authors proved that this index can significantly enhance the physico-chemical applicability of the first Zagreb index. We refer to [3] for more information about this graph invariant.

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The real number $\lambda$is called the eigenvalue of a graph Γ with adjacency matrix Aif the equation $Ax=\lambda x$has a nonzero solution. A solution $v$for this equation is called eigenvector corresponding to the eigenvalue λ. The characteristic polynomial of the matrix A is defined as$\chi_\lambda(G) = det(A - \lambda I)$. It is easy to see that the eigenvalues of A are roots of$\chi_\lambda(G)$.

2. NOTATION AND DEFINITIONS

There are two types of Zagreb indices introduced by Gutman and Trinajestic[12]: the first Zagreb index M_1 and the second Zagreb index M_2 defined as follows:

$$M_1 = M_1(G) = \sum_{u\in V(G)} d(u)^2 \text{ and } M_2 = M_2(G) = \sum_{uv\in E(G)} d(u)d(v),$$

where d_u denotes the degree of vertex u, see [1,4,7,9]. The first Zagreb index can be rewritten also as $M_1 = M_1(G) = \sum_{uv\in E(G)}[d(u) + d(v)]$. For more details on these topological indices we refer to [7, 14–16, 18]. With this notation, the F- index is defined as [2,3,11,13]

$$F = F(G) = \sum_{u\in V(G)} d(u)^3 = \sum_{uv\in E(G)}[d(u)^2 + d(v)^2].$$

In [5] the following three topological indices are proposed:

$$TI_1 = TI_1(G) = \sum_{v\in V(G)} F_1(v), TI_1 = TI_1(G) = \sum_{uv\in E(G)} F_2(u.v),$$
$$TI_1 = TI_1(G) = \sum_{u\neq v.\{u.v\}\subseteq V(G)} F_3(u.v) \qquad (1)$$

where F_1, F_2 and F_3 are functions dependent of a vertex or on a pair of vertices of the molecular graph G and forgotten index is of the form *Equation* 1.

3. BOUNDS OF FORGOTTEN INDEX

Let G be a graph on n vertices with maximum degree Δ, where $n \geq 3$. It is clear that $5m \leq d_u^2 + d_v^2 \leq 2\Delta^2$ and thus $5m \leq F(G) \leq 2\Delta^2 m$. The aim of this section is to compute some bounds for $F(G)$ and then we present some algebraic properties of this index. Let A be the adjacency matrix of G and B is a symmetric matrix with the following entries:

$$b_{uv} = \begin{cases} d(u)^2 + d(v)^2 & if\ uv \in E(G) \\ 0 & otherwise \end{cases}.$$

Lemma 2. We have

i) $F(G) \leq \sqrt{tr(A^2)m/2}$,

ii) $\sum_{uv\in E(G)} d_u^2 d_v^2 \geq M_1^2(G)/n$,

iii) $tr(B) = 2$ and $\sum_{uv\in E(G)}(d_u^2 + d_v^2)^2$,

iv) $F(G) \geq \sqrt{\frac{tr(B^2)}{2}}$,

v) If G is r-regular, then $F(G) = \frac{1}{4r^2} tr(B^2)$.

Proof.

i) It is not so difficult to see that

$$F(G) = \sum_{uv\in E(G)}[d_u{}^2 + d_v{}^2] \leq \sqrt{\sum_{uv\in E(G)}(d_u{}^2 + d_v{}^2)^2} \cdot m^{\frac{1}{2}} = \sqrt{tr(A^2)m/2},$$

as desired.

ii) According to geometrical-arithmetic inequality we have

$$M_1^2(G) = \left(\sum_{u\in V(G)} d_u^2\right)^2 \geq n \sum_{uv\in E(G)} d_u^2 d_v^2.$$

iii) Since every element in the main diagonal of B is 0, we obtain $tr(B)$=0 The i-th entry b_{ii} in the diagonal of B^2 is $b_{ii} = \sum_{v_iv_j\in E(G)} \left[d_{v_i}{}^2 + d_{v_j}{}^2\right]^2$. Thus, $tr(B^2)$ $= \sum_{i=1}^n b_{ii} = \sum_{i=1}^n \sum_{u_iv_i\in E(G)} \left(d_{v_i}{}^2 + d_{v_j}{}^2\right)^2 = 2\sum_{uv\in E(G)}(d_u{}^2 + d_v{}^2)^2$.

iv) By Lemma 1, $tr(B^2) = 2\sum_{uv\in E(G)}(d_u{}^2 + d_v{}^2)^2 \leq 2\sum_{uv\in E(G)}(d_u{}^2 + d_v{}^2)\sum_{uv\in E(G)}(d_u{}^2 + d_v{}^2) \leq 2F^2(G)$.

v) If G is r-regular, then $B = 2r^2A$ and $tr(B^2) = 4r^4 tr(A^2)$. Hence,

$$F(G) = 2r^2m = 2r^2 \times \frac{1}{2} tr(A^2) = \frac{1}{4r^2} tr(B^2).$$

Denote by σ^2 the variance of the sequence of the terms $\{d_u{}^2 + d_v{}^2\}$ appearing in the definition of $F(G)$.

Lemma 3. For any graph G, $F(G) = \sqrt{m/2tr(B^2) - m^2\sigma^2}$.

Proof. Lemma 2 gives $\frac{1}{2} tr(B^2) = \sum_{uv\in E(G)}(d_u{}^2 + d_v{}^2)^2$. By the definition of σ^2, we have

$$\sigma^2 = \frac{1}{m}\sum_{uv\in E(G)}(d_u{}^2 + d_v{}^2)^2 - \left(\frac{1}{m}\sum_{uv\in E(G)}(d_u{}^2 + d_v{}^2)\right)^2 = \frac{1}{2m} tr(B^2) - \frac{1}{m^2}F(G)^2$$

and this equality yields the results.

Lemma 4. Let $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$ be all eigenvalues of B, then we have

i) $\sum_{i=1}^n \mu_i^2 \geq n\mu_1^2/(n-1)$.

ii) $\sqrt{\frac{n}{2(n-1)}}\mu_1 \leq F(G) \leq \frac{1}{2}\mu_1 n$.

Proof. Suppose $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$ are the eigenvalues of B.

i) Since $\sum_{i=1}^{n}\mu_i = tr(B) = 0$, we have $\mu_1 = -\sum_{i=2}^{n}\mu_i$ and Cauchy-Schwarz inequality gives

$$\mu_1^2 = (\sum_{i=2}^{n}\mu_i)^2 \le (\sum_{i=2}^{n}\mu_i)^2(n-1).$$

Hence,

$$\sum_{i=1}^{n}\mu_i^2 = \mu_1^2 + \sum_{i=2}^{n}\mu_i^2 \ge \mu_1^2 + \frac{\mu_1^2}{n-1} = \frac{n\mu_1^2}{n-1}.$$

ii) Suppose *j* is the vector $j = (1.1.\dots 1) \in R^n$. By Perron-Frobenius theorem we can conclude that $\mu_1 \ge |\mu_j|$, for every *j*, and then $\mu_1 \ge 0$. Hence, Rayleigh quotient yields

$$\mu_1 = max\frac{\langle Bx.x\rangle}{\|x\|^2} \ge \frac{\langle Bj.j\rangle}{\|j\|^2} = \frac{2F(G)}{n}.$$

According to Part (i), we have

$$F(G)^2 = \left(\sum_{uv\in E(G)}\left({d_u}^2 + {d_v}^2\right)\right)^2 \ge \sum_{uv\in E(G)}\left({d_u}^2 + {d_v}^2\right) \ge \frac{1}{2}\sum_{i=1}^{n}\mu_i^2$$
$$= \frac{1}{2}(\mu_1^2 + \sum_{i=2}^{n}\mu_i^2) \ge \frac{1}{2}\left(\mu_1^2 + \frac{\mu_1^2}{n-1}\right) = \frac{n\mu_1^2}{2(n-1)}.$$

Assume now that *G* is a Δ-regular graph. Then $B = 2\Delta^2 A$ and $\mu_i = 2\Delta^2\lambda_i$. It is well know that the greatest eigenvalue of a Δ-regular graph is Δ itself. Hence, $\mu_1 = 2\Delta^2\lambda_1$ and then $F(G) = 2\Delta^2 m = \Delta^2\Delta n = n\Delta^2\lambda_1 = \frac{n}{2}\mu_1$.

4. SPECTRAL PROPERTIES

For given graph *G*, if the maximum degree of every vertex reaches to four, then *G* is called a molecular graph. The first **inverse sum indeg index** (ISI index) defined as follows [17]:

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

Let V(*G*)= {$v_1,v_2,\dots,v_n$} 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 a matrix with entries b_{ij} as follows:

$$b_{ij} = \begin{cases} \frac{d_i d_j}{d_i + d_j} & v_i v_j \in E(G) \\ 0 & otherwise \end{cases}.$$

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

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

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

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

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

The diagonal elements of PA^2 are $\frac{4}{9}.\frac{13}{9}.2.2.\dots.2.\frac{13}{9}.\frac{4}{9}$. Therefore,

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

Lemma 4. Let $PA(G) = \frac{r}{2}A(G)$, then $\chi_\lambda\big(PA(G)\big) = (\frac{r}{2})^n\chi_{\frac{2}{r}\lambda}\big(A(G)\big)$.

Proof. The proof is straightforward.

For an example, $PA(S_n) = \frac{n-1}{n}A(S_n)$ and by using Lemma 4,

$$\chi_\lambda\big(PA(S_n)\big) = (\frac{n-1}{n})^n\chi_{\frac{n\lambda}{n-1}}\big(A(S_n)\big).$$

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

$$\chi_\lambda\big(PA(K_{m.n})\big) = (\frac{mn}{m+n})^n\chi_{\frac{(m+n)\lambda}{mn}}\big(A(K_{m.n})\big).$$

Theorem 5. Let *G* be a graph with vertices set $\{1.2.\dots.n\}$ and *ISI* matrix PA. Then

i) $tr(PA) = 0$

ii) $tr(PA^2) = 2\sum_{i\sim j}\left(\frac{d_id_j}{d_i+d_j}\right)^2 .\ (PA^2)_{jj} = d_id_j\sum_{.k\sim i.k\sim j}\frac{d_k^2}{(d_i+d_k)(d_j+d_k)}$.

iii) $tr(PA^3) = 2\sum_{i\sim j}\frac{(d_id_j)^2}{d_i+d_j}\left(\sum_{.k\sim i.k\sim j}\frac{d_k^2}{(d_i+d_k)(d_j+d_k)}\right)$.

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

Proof. All parts can be proved as follows:

i) The Part (i) is clear.

ii) For *i=j*, $(PA^2)_{ii} = \sum_{k=1}^n PA_{ik}PA_{ki} = \sum_{k=1}^n(PA_{ik})^2 = \sum_{i\sim j}(PA_{ij})^2 = \sum_{i\sim j}\left(\frac{d_id_j}{d_i+d_j}\right)^2$. Therefore, $tr(PA^2) = \sum_{i=1}^n\sum_{i\sim k}\left(\frac{d_id_k}{d_i+d_k}\right)^2 = 2\sum_{i\sim j}\left(\frac{d_id_j}{d_i+d_j}\right)^2$. Suppose *i≠j*. Then, $(PA^2)_{ij} = \sum_{k=1}^n PA_{ik}PA_{kj} = \sum_{.k\sim i.k\sim j}PA_{ik}PA_{kj} = \sum_{.k\sim i.k\sim j}\left(\frac{d_id_k}{d_i+d_k}\right)\left(\frac{d_jd_k}{d_j+d_k}\right) = d_id_j\sum_{.k\sim i.k\sim j}\frac{d_k^2}{(d_i+d_k)(d_j+d_k)}$.

iii) For the matrix PA^3 we have $(PA^3)_{ii} = \sum_{j=1}^{n} PA_{ij}(PA^2)_{jk} = \sum_{i\sim j} \frac{d_i d_j}{d_i+d_j}(PA^2)_{jk} = \sum_{i\sim j}(\sum_{.k\sim i.k\sim j} \frac{d_k^2}{(d_i+d_k)(d_j+d_k)})$ and so we obtain

$$tr(PA^3) = \sum_{i=1}^{n}\sum_{i\sim j} \frac{(d_i d_j)^2}{d_i+d_j}(\sum_{.k\sim i.k\sim j} \frac{d_k^2}{(d_i+d_k)(d_j+d_k)})$$
$$= 2\sum_{i\sim j} \frac{(d_i d_j)^2}{d_i+d_j}(\sum_{.k\sim i.k\sim j} \frac{d_k^2}{(d_i+d_k)(d_j+d_k)}).$$

iv) The trace of PA^4 is

$$tr(PA^4) = \sum_{i.j=1}^{n}(PA^2)_{ij}^2 = \sum_{i=j}(PA^2)_{ij}^2 + \sum_{i\neq j}(PA^2)_{ij}^2$$
$$= \sum_{i=1}^{n}\left(\sum_{i\sim l}\left(\frac{d_i d_l}{d_i+d_l}\right)^2\right)^2 + \sum_{i\neq j} d_i d_j (\sum_{.l\sim i.l\sim j} \frac{d_l^2}{(d_i+d_l)(d_j+d_l)})^2.$$

This completes our argument.

5. ENERGY AND LAPLACIAN ENERGY

One of branches of graph theory which has many applications in chemistry is spectral theory based on the eigenvalues of the adjacency matrix [6,10]. Let *G* be a simple graph on *n* vertices and $\lambda_1.\lambda_2.\dots.\lambda_n$ be the eigenvalues of its adjacency matrix. The energy *E*(*G*) of the graph *G* is defined as the sum of the absolute values of its eigenvalues, i.e. $E = E(G) = \sum_{i=1}^{n}|\lambda_i|$. Here, we define the ISI energy as the sum of absolute values of the eigenvalues of the ISI matrix. More formally: Let $\rho_1.\rho_2.\dots.\rho_n$ be the eigenvalues of the ISI matrix PA(*G*). It is not difficult to see that these eigenvalues are real numbers and their sum is zero. Hence, the ISI energy can be defined as [8] $PAE = PAE(G) = \sum_{i=1}^{n}|\rho_i|$. This definition is applicable to all graphs.

Theorem 6. Let *G* be a graph with *n* vertices. Then $PAE(G) \leq \sqrt{2n}ISI(G)$.

Proof. The variance of the numbers $|\rho_i|$, *i*=1,2,…,*n* is equal to

$$\frac{1}{n}\sum_{i=1}^{n}|\rho_i|^2 - \left(\frac{1}{n}\sum_{i=1}^{n}|\rho_i|\right)^2$$

which is greater than or equal to zero. Now, $\sum_{i=1}^{n}|\rho_i|^2 = \sum_{i=1}^{n}\rho_i{}^2 = tr(PA^2)$ and therefore $\frac{1}{n}tr(PA^2) - (\frac{1}{n}PAE)^2 \geq 0$. Hence,

$$PAE(G) \leq \sqrt{ntr(PA^2)} \leq \sqrt{2n(ISI(G))^2} = \sqrt{2n}ISI(G).$$

Theorem 7. Let *G* be a graph with *n* vertices and at least one edge. Then

$$PAE(G) \geq 2\sum_{i\sim j}\frac{d_id_j}{d_i+d_j}\left(\frac{2\sum_{i\sim j}\frac{d_id_j}{d_i+d_j}}{\sum_{i=1}^{n}\left(\sum_{i\sim j}\left(\frac{d_id_j}{d_i+d_j}\right)^2\right)^2+\sum_{i\neq j}d_id_j\left(\sum_{k\sim i,k\sim j}\frac{d_k^2}{(d_i+d_k)(d_j+d_k)}\right)^2}\right)^{\frac{1}{2}}.$$

Proof. The Hölder inequality implies that

$$\sum_{i=1}^{n}a_ib_i \leq \left(\sum_{i=1}^{n}a_i^p\right)^{1/p}\left(\sum_{i=1}^{n}a_i^q\right)^{1/q}$$

which holds for any non-negative real number a_i, $b_i(i = 1,2,\ldots,n)$. Put $a_i = |\rho_i|^{2/3}$, $b_i = |\rho_i|^{4/3}$, $p = 3/2$ and $q = 3$, thus we have

$$\sum_{i=1}^{n}|\rho_i|^2 = \sum_{i=1}^{n}|\rho_i|^{2/3}(|\rho_i|^4)^{1/3} \leq \left(\sum_{i=1}^{n}|\rho_i|\right)^{2/3}\left(\sum_{i=1}^{n}|\rho_i|^4\right)^{1/3}. \quad (3)$$

If *G* has at least one edge, then not all ρ_i's are equal to zero. Then $\sum_{i=1}^{n}|\rho_i^4| \neq 0$ and Equation 3 can be rewritten as

$$PAE(G) = \sum_{i=1}^{n}|\rho_i| \geq \frac{\left(\sum_{i=1}^{n}|\rho_i|^2\right)^{\frac{3}{2}}}{\left(\sum_{i=1}^{n}|\rho_i^4|\right)^{\frac{1}{2}}} = \frac{\left(\sum_{i=1}^{n}\rho_i^2\right)^{\frac{3}{2}}}{\left(\sum_{i=1}^{n}\rho_i^4\right)^{\frac{1}{2}}} = \sqrt{\frac{tr(PA^2)^3}{tr(PA^4)}}$$

$$= 2\sum_{i\sim j}\frac{d_id_j}{d_i+d_j}\left(\frac{2\sum_{i\sim j}\frac{d_id_j}{d_i+d_j}}{\sum_{i=1}^{n}\left(\sum_{i\sim j}\left(\frac{d_id_j}{d_i+d_j}\right)^2\right)^2+\sum_{i\neq j}d_id_j\left(\sum_{k\sim i,k\sim j}\frac{d_k^2}{(d_i+d_k)(d_j+d_k)}\right)^2}\right)^{\frac{1}{2}}.$$

Theorem 8. If *G* is a regular graph of degree *r* where *r*>0, then $PAE(G) = \frac{r}{2}E(G)$. If, in addition *r* = 0, then PA*E* = 0.

Proof. If $r = 0$, then *G* is a graph without edges. Then directly from the definition of matrix *PA*, it follows that $PA_{ij} = 0$, for all $i,j = 1,2,\ldots,n$ and consequently PA(*G*) = 0. Therefore, PA*E*(*G*) = 0. Suppose now that *G* is regular of degree $r \geq 0$ and $d_1 = d_2 = \cdots = d_n = r$. Then all none-zero terms in PA(*G*) are equal to *r*/2, implying that $PA(G) = \frac{r}{2}A(G)$. Therefore, $\rho_i = \frac{r}{2}\lambda_i$ for *i*=1,2,…*n* and hence $PAE(G) = \sum_{i=1}^{n}|\rho_i| = \frac{r}{2}\sum_{i=1}^{n}|\lambda_i| = \frac{r}{2}E(G)$, which completes the proof.

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