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# On the topological matrix and topological indices

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## Abstract

The topological matrix  $M$  of a graph  $G$  are indexed by  $V(G)$ . If  $i, j \in L$  then the  $(i, j)$  – entry of  $M(G)$  is 1 and the  $(i, j)$  – entry of  $M(G)$  is 0 for otherwise. In this paper, an upper bound for this topological matrix is found and the weighted topological matrix is defined. Also, some inequalities for the topological energy and the weighted Laplacian topological energy and of  $M(G)$  are obtained.

The Topological index  $TI(G)$  of a graph  $G$  is qualified by  $TI = |A + D|$ . Some relations are found for basic mathematical operations of  $TI(G)$  and some bounds are reported for some topological indices in this paper.

*Keywords:* Topological matrix; Topological indices; Bounds

## 1. Introduction

Let  $G$  be a simple connected graph on the vertex set  $V(G)$  and the edge set  $E(G)$ . If  $v_i$  and  $v_j$  are adjacent, then we use the notation  $v_i \sim v_j$ . For  $v_i \in V(G)$ , the degree of  $v_i$ , denoted by  $d_i$  is the number of the vertices adjacent to  $v_i$ . Let  $A(G)$  be adjacency matrix of  $G$  and  $\lambda_1, \lambda_2, \dots, \lambda_n$  be its eigenvalues ( $\lambda_1$  is the greatest eigenvalue). The graph eigenvalues provide these well-known results:  $\sum_{i=1}^n \lambda_i = 0$ ,  $\sum_{i=1}^n \lambda_i^2 = 2m$ ,  $\lambda_1 \geq \frac{2m}{n}$  [1,2]. In this paper, the reciprocals of the graph indices are examined under these basic concepts. The graph indices which is one of the topics involved in the studies of graph theory. An important part of these graph indices is topological indices that is used in chemical graph theory, particularly. Chemical graph theory can make topological representation of a molecule. The numerical values of this chemical structure are descriptors. A topological index is calculated from a graph representing a molecule and this index is also invariant number of graphs. Most recommended topological indices consists of vertex, edge, degree relationship. This, describes the atomic relationship in chemical graph theory. This means that, graph theory contributes organic compounds with calculations and creating diagrams. This paper indicates special bounds for some topological indices by the help of different mathematical formulas and series. These topological indices are described as follows:

Let  $A$  be an adjacency matrix and  $D$  be a graph distance matrix. The topological index defined by

$$TI = |A + D|$$

where  $|A + D|$  denotes the determinant of the matrix addition.

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The atom-bond connectivity index  $ABC$  is one of the popular degree-based topological indices in chemical graph theory [3] such that

$$ABC = ABC(G) = \sum_{v_i v_j \in E(G)} \sqrt{\frac{d_i + d_j - 2}{d_i d_j}}.$$

Randić index is a well known topological structure such that

$$R(G) = \sum_{v_i v_j \in E(G)} \frac{1}{\sqrt{d_i d_j}}.$$

It is referred that the articles [4] and [5] for the various properties on the Randić index. Another remarkable topological descriptor is the Harmonic index, characterized in [6] as

$$H(G) = \sum_{v_i v_j \in E(G)} \frac{2}{d_i + d_j}.$$

Recently [7], a graph invariant came into the focus of attention, defined as

$$F = F(G) = \sum_{i=1}^n d_i^3$$

which for historical reasons [8] was named forgotten topological index.  $F$  satisfies the identities

$$F(G) = \sum_{i \sim j} d_i^2 + d_j^2.$$

One of the aim of this paper is to define the weighted topological matrix of a graph and to provide upper bounds on the weighted topological matrix  $M_{ij}$  and the eigenvalues of the graph  $G$ . It is needed that the following results in order to effect these bounds:

The Topological matrix  $M_{ij}$  of a graph  $G$  is defined by

$$M_{ij}^w = \begin{cases} 1 & ; \quad i, j \in L \\ 0 & ; \quad \text{otherwise.} \end{cases} \quad (1.1)$$

where  $L$  is a link.

Let  $\lambda_1(M)$  be greatest eigenvalue and  $M = (m_{ij})$  be an  $n \times n$  irreducible nonnegative matrix. Let  $R_i(M) = \sum_{j=1}^n m_{ij}$  [9]. Then,

$$(\min R_i(M) : 1 \leq i \leq n) \leq \lambda_1(M) \leq (\max R_i(M) : 1 \leq i \leq n). \quad (1.2)$$

Let  $V$  be a vertex set,  $v_i \in V$  and  $e_i$  be an average degree. If  $G$  is a simple, connected graph then [10]

$$\lambda_1(G) \leq \max(\sqrt{e_i e_j} : 1 \leq i, j \leq n, v_i, v_j \in E) \quad (1.3)$$

The energy of a graph  $G$  is described as  $E(G) = \sum_{i=1}^n |\lambda_i|$  where  $\lambda_i, i = 1, 2, \dots, n$  are the eigenvalues of graph  $G$ . The Laplacian energy of a graph  $G$  is qualified as  $LE(G) = \sum_{i=1}^n |\mu_i - \frac{2m}{n}|$  where  $\mu_i, i = 1, 2, \dots, n$  are the laplacian eigenvalues of graph  $G$  [2,11].

**Lemma 1.1.** [11] Let  $a_i, b_i \in R$  and  $a, b, A, B$  be real constants such that  $i = 1, 2, \dots, n, 0 < a \leq a_i \leq A$  and  $0 < b \leq b_i \leq B$ . Then,

$$|n \sum_{i=1}^n a_i b_i - \sum_{i=1}^n a_i \sum_{i=1}^n b_i| \leq \alpha(n)(A - a)(B - b)$$

where  $\alpha(n) = n \lfloor \frac{n}{2} \rfloor \left( \left[ 1 - \frac{1}{n} \right] \lfloor \frac{n}{2} \rfloor \right)$ .

See [1,12–16] for details about graph theory and topological structures.

The scheme of the paper is as follows: In Section 1, a list of some previously known definitions and results are introduced. In Section 2, a new topological matrix and topological energy are defined for the weighted graphs. Also, some relations are established in terms of edges, vertices and degrees. In addition, different relationships are obtained for topological indices.

## 2. Main results

### 2.1. On the topological matrix

In this section, the weighted Topological matrix and the weighted Topological energy are defined. Furthermore, a relationship is found between the weighted Topological energy and the eigenvalues of the weighted Topological matrix.

**Definition 2.1.** Let  $G$  be a simple, connected, edge weighted graph. The weighted Topological matrix  $M^w = M^w(G)$  of  $G$  defined by,

$$M_{ij}^w = \begin{cases} w_{ij} & ; \quad i, j \in L \\ 0 & ; \quad \text{otherwise.} \end{cases} \tag{2.1}$$

where  $w(u) = \sum_{i \sim u} t_i$ ,  $w(v) = \sum_{j \sim v} c_j$ .

The weighted Topological eigenvalues  $\rho_1^w, \rho_2^w, \dots, \rho_n^w$  are the eigenvalues of its weighted Topological matrix  $M^w$ . These eigenvalues can be put in order such that  $\rho_1^w \geq \rho_2^w \geq \dots \geq \rho_n^w$ .

**Definition 2.2.** Let  $G$  be a simple, connected weighted graph with  $n$  vertex. Let  $G$  be edge weighted graph and these weights be positive real numbers. The weighted Topological energy  $ME = ME(G_w)$  of  $G_w$  is defined as follows:

$$ME = ME(G_w) = \sum_{i=1}^n |\rho_i^w| \tag{2.2}$$

where  $\rho_i^w$  is the eigenvalue of weighted Topological matrix  $M^w$ .

**Definition 2.3.** Let  $G$  be a simple, connected weighted graph. The weighted Laplacian Topological energy  $LME = LME(G_w)$  of  $G_w$  is defined as follows:

$$ME = ME(G_w) = \sum_{i=1}^n \left| \rho_i^w - \frac{2m}{n} \right| \tag{2.3}$$

where  $\rho_i^w$  is the laplacian eigenvalue of weighted Topological matrix  $M^w$ .

**Theorem 2.4.** If  $G$  is a simple, connected graph of  $M$ , then

$$\lambda_1(G) \leq \frac{2e}{d_1}$$

where  $d_1$  is the degree of  $G$ .

**Proof.** Let multiply the topological matrix with the diagonal matrix and the inverse of diagonal matrix. Let show this multiplication by  $D(G)^{-1}M(G)D(G)$ . Let consider an eigenvector of  $D(G)^{-1}M(G)D(G)$  and this eigenvector be  $X = (x_1, x_2, \dots, x_n)^T$ . Let one eigencomponent  $x_i = 1$  and the other eigencomponent  $0 < x_k \leq 1$  for every  $k$ . Let  $x_j = \max_k(x_k : v_i v_k \in E, i \sim k)$ . It is known that

$$(D(G)^{-1}M(G)D(G))X = \lambda_1(G)X. \text{ It is implies that } \lambda_1(G)x_i = \sum_k (m_{1k} \frac{d_k}{d_1})x_k. \text{ Since } (1, k) \in L \text{ then,}$$

$$\lambda_1(G)x_i = \frac{1}{d_1} \sum_k (d_k)x_k. \text{ It is well known that } \sum_{i=1}^n d_i = 2e. \text{ Thus, } \lambda_1(G) \leq \frac{2e}{d_1}. \text{ From (1.3), the inequality}$$

results that  $\lambda_1(G) \leq \frac{2e}{d_1}$ .  $\square$

**Corollary 2.5.** Let  $G$  has  $n$  vertices and  $m$  edges. Let  $\bar{G}$  be the complement of a graph  $G$ . If  $G$  and  $\bar{G}$  be connected non-singular graphs of  $M$  then,

$$\lambda_1(G) - \lambda_1(\bar{G}) \leq \frac{(n - 1)(2e - nd_1)}{(n - 1 - d_1)d_1}.$$

**Proof.** Using Theorem 2.4,

$$\lambda_1(G) - \lambda_1(\bar{G}) \leq \frac{2e}{d_1} - \frac{2\bar{e}}{n-1-d_1}.$$

Since,  $2e + 2\bar{e} = n(n-1)$ , then

$$\lambda_1(G) - \lambda_1(\bar{G}) \leq \frac{(n-1)(2e - nd_1)}{(n-1-d_1)d_1}. \quad \square$$

**Theorem 2.6.** Let  $G$  be a simple, connected graph with  $m$  edges and  $ME(G)$  be a Topological energy of  $G$  then,

$$|ME(G) + ME(G - e)| \leq \sqrt{4m + 4\sqrt{m(m - \delta)}}.$$

**Proof.** Let  $\lambda_i$  be  $i$ -th eigenvalue of  $M(G)$ . Define  $\lambda'_i = \lambda_i(G - e)$ . It is known that  $ME(G) = \sum_{i=1}^n |\lambda_i|$ . Since  $\sum_{i=1}^n (\lambda_i)^2 = 2m$  and  $\sum_{i=1}^n (\lambda'_i)^2 = 2(m - \delta)$  then,

$$\sum_{i=2}^n (|\lambda_i| + |\lambda'_i|)^2 \leq 2m - (\lambda_1)^2 + 2m - 2\delta - (\lambda_1)^2 \tag{2.4}$$

$$+ 2\sqrt{(2m - (\lambda_1)^2)(2m - 2\delta - (\lambda_1)^2)} \tag{2.5}$$

$$\leq 4m - \frac{4m^2}{n^2} + \frac{4m^2 - 4m\delta - 4\delta^2}{n^2 - 2n + 1} + 2\sqrt{(2m - \frac{4m^2}{n^2})(2m - 2\delta - \frac{4m^2}{n^2})}. \tag{2.6}$$

This means that,

$$ME(G) + ME(G - e) \leq |\lambda_1| + |\lambda'_1| + \sum_{i=2}^n |\lambda_i| + \sum_{i=2}^n |\lambda'_i| \tag{2.7}$$

$$\leq |\lambda_1| + |\lambda'_1| \tag{2.8}$$

$$+ \sqrt{4m - \frac{4m^2}{n^2} + \frac{4m^2 - 4m\delta - 4\delta^2}{n^2 - 2n + 1} + 2\sqrt{(2m - \frac{4m^2}{n^2})(2m - 2\delta - \frac{4m^2}{n^2})}. \tag{2.9}$$

Since  $|\lambda_1| \geq \frac{2m}{n}$  and  $|\lambda'_1| \geq \frac{2(m-\delta)}{n-1}$ , the inequality turns into

$$ME(G) + ME(G - e) \leq \frac{2m}{n} + 2\frac{(m - \delta)}{n - 1} \tag{2.10}$$

$$+ \sqrt{4m - \frac{4m^2}{n^2} + \frac{4m^2 - 4m\delta - 4\delta^2}{n^2 - 2n + 1} + 2\sqrt{(2m - \frac{4m^2}{n^2})(2m - 2\delta - \frac{4m^2}{n^2})}. \tag{2.11}$$

It is constructed a sequence  $G_n (n \geq 2)$  of graphs to complete the argument such that  $|ME(G_n) + ME(G_n - e)| \rightarrow \sqrt{4m + 4\sqrt{m(m - \delta)}}$ . This completes argument.  $\square$

**Theorem 2.7.** Let  $G_w$  be a weighted graph with  $n$  vertices and  $m$  edges. Let  $\rho_1^w \geq \rho_2^w \geq \dots \geq \rho_{k-1}^w \geq \rho_k^w (k \leq n)$  be  $k$  non-zero laplacian eigenvalues of the weighted Topological matrix and  $MLE(G_w)$  be a Topological Laplacian energy of  $G_w$  then,

$$|MLE(G_w)| \geq \sqrt{(\frac{2m(n-1)}{n})^2 k - \alpha(k) |\rho_1^w - \rho_k^w|^2}.$$

where  $\alpha(k) = k[\frac{k}{2}][1 - \frac{1}{k}][\frac{k}{2}]$  while  $[x]$  denotes integer part of a real number  $x$ .

**Proof.**

If  $MLE(G_w)$  is a weighted Topological Laplacian energy of  $G_w$  then,  $MLE(G_w) = \sum_{i=1}^k |\rho_i^w - \frac{2m}{n}|$  and

$$\sum_{i=1}^k |\rho_i^w - \frac{2m}{n}|^2 = \sum_{i=1}^n |\rho_i^w - \frac{2m}{n}|^2 = \sum_{i=1}^n (\rho_i^w - \frac{2m}{n})^2. \tag{2.12}$$

Seeing that,

$$\sum_{i=1}^n (\rho_i^w - \frac{2m}{n})^2 = \sum_{i=1}^n ((\rho_i^w)^2 - \frac{4m}{n} \rho_i^w + \frac{4m^2}{n^2}) \tag{2.13}$$

$$= (2m)^2 - \frac{8m^2}{n} + \frac{4m^2}{n^2}. \tag{2.14}$$

It requires that,

$$\sum_{i=1}^k |\rho_i^w - \frac{2m}{n}|^2 = 4m^2 - \frac{8m^2}{n} + \frac{4m^2}{n^2}. \tag{2.15}$$

Setting  $a_i = |\rho_i^w - \frac{2m}{n}|$ ,  $b_i = |\rho_i^w - \frac{2m}{n}|$ ,  $a = b = |\rho_1^w - \frac{2m}{n}|$  and  $A = B = |\rho_1^w - \frac{2m}{n}|$ ,  $i = 1, 2, \dots, k$ .

Lemma 1.1 becomes

$$|k \sum_{i=1}^k |\rho_i^w - \frac{2m}{n}|^2 - (\sum_{i=1}^k |\rho_i^w - \frac{2m}{n}|)^2| \leq \alpha(k) (|\rho_1^w - \frac{2m}{n}| - |\rho_k^w - \frac{2m}{n}|)^2. \tag{2.16}$$

Thus, the inequality transforms into

$$(4m^2 - \frac{8m^2}{n} + \frac{4m^2}{n^2})k - (MLE(G_w))^2 \leq \alpha(k) |\rho_1^w - \rho_k^w|^2. \tag{2.17}$$

Hence,

$$|MLE(G_w)| \geq \sqrt{(\frac{2m(n-1)}{n})^2 k - \alpha(k) |\rho_1^w - \rho_k^w|^2}. \quad \square$$

### 2.2. Some notes on the topological indices

In this section, some results are given for Topological indices of graph operations. These results are obtained in terms of Topological indices and in fact, the bounds are tight. Also, upper bounds on the some topological indices are determined involving just the forgotten topological index, the Randić index, the ABC index, the Harmonic index and the edges.

**Theorem 2.8.** *Let G and H be two simple graph and  $E_G, E_H$  be edge sets,  $V_G, V_H$  be vertex sets, respectively. Then,*

- (1)  $TI(G + H) = (-1)^{V^+-1} (V^+ - 1) 2^{V^+}$ .
- (2)  $TI(G \cup H) = (-1)^{V^\cup-1} (V^\cup - 1) 2^{V^\cup}$ .
- (3)  $TI(G \cap H) = (-1)^{V^\cap-1} (V^\cap - 1) 2^{V^\cap}$ .

where  $|V_G + V_H| = V^+$ ,  $|V_G \cup V_H| = V^\cup$  and  $|V_G \cap V_H| = V^\cap$ .

**Proof.** (1) Let  $E_G$  and  $E_H$  be edge sets,  $V_G, V_H$  be vertex sets,  $V = V_G \cup V_H$ ,  $E = E_G \cup E_H \cup \{(u_G, u_H) \mid u_G \in V(G), u_H \in V(H)\}$ . It is obvious from the definition,

$$TI(G + H) = (-1)^{V^+-1} (V^+ - 1) 2^{V^+}.$$

(2) Let denote  $G = G \times H$  edge sets. To define the product  $G \times H$  of two graphs think any two points  $u = (u_G, u_H)$  and  $v = (v_G, v_H)$  and  $u, v \in V = V_G \times V_H$ . Hence,  $u$  and  $v$  are adjacent in  $G \times H$  whenever  $[u_G = v_G$  and  $u_H$  adjacent to  $v_H]$  or  $[u_H = v_H$  and  $u_G$  adjacent to  $v_G]$ . Then,

$$TI(G \cup H) = (-1)^{V^\cup-1} (V^\cup - 1) 2^{V^\cup}.$$

(3) If two graphs  $G$  and  $H$  have at least one common vertex then their intersection will be a graph such that  $V(G \cap H) = V(G) \cap V(H)$  and  $E(G \cap H) = E(G) \cap E(H)$ . Hence,

$$TI(G \cap H) = (-1)^{V^\cap-1} (V^\cap - 1) 2^{V^\cap}. \quad \square$$

**Theorem 2.9.** Let  $G$  and  $H$  be two simple graphs. If  $G$  and  $H$  are isomorph then topological indices of  $G$  and  $H$  are equal.

**Proof.** Let  $V_G$  and  $V_H$  be vertex sets of  $G$  and  $H$ , respectively. Let  $E_G$  and  $E_H$  be edge sets of  $G$  and  $H$ , respectively. Since  $G$  and  $H$  are isomorph graphs then  $V_G = V_H$  and  $E_G = E_H$ . Thus, the adjacency matrix and the distance matrix of these graphs are equal that is ;  $A(G) = A(H)$  and  $D(G) = D(H)$ . It is seen that  $TI(G) = TI(H)$ .  $\square$

Furthermore, some formulas for Topological index of popular graphs are obtained, directly. Let  $K_n$ ,  $P_n$ ,  $C_n$  and  $S_n$  show the  $n$ -vertex complete graph, path, cycle and star graph, respectively.

**Corollary 2.10.**

Let  $G$  be a simple connected graph with  $n$  vertices. Then,

(1) For  $2 \leq n \leq 6$ ,

$$TI(K_n) = TI(C_n) = TI(S_n).$$

(2) For  $2 \leq n \leq 3$ ,

$$TI(K_n) = TI(C_n) = TI(S_n) = TI(P_n).$$

(3) For  $n \geq 2$ ,

$$TI(K_n) = TI(S_n) = (-1)^{n-1}(n-1)2^n.$$

**Theorem 2.11.** Let  $G$  be a connected graph with  $m$  edges, then

$$4H_{-1}(G) - F(G) - 2R_{-1}^2(G) \leq 2\sqrt{m(F(G) + 2R_{-1}^2(G))}.$$

**Proof.** Minkowski inequality gives

$$\left( \sum_{v_i v_j \in E(G)} (d_i + d_j + 1)^2 \right)^{\frac{1}{2}} \leq \left( \sum_{v_i v_j \in E(G)} (d_i + d_j)^2 \right)^{\frac{1}{2}} + \left( \sum_{v_i v_j \in E(G)} 1 \right)^{\frac{1}{2}}.$$

In the Bernoulli inequality,  $(1+x)^\alpha$  is greater than or equal to  $1+\alpha x$  for  $x \geq -1$ . It gives  $(1+d_i+d_j)^2 \geq 1+2(d_i+d_j)$ . Hence,  $\sum_{v_i v_j \in E(G)} (1+2(d_i+d_j)) = m+2\sum_{v_i v_j \in E(G)} (d_i+d_j)$ . It follows that,

$$(m+2 \sum_{v_i v_j \in E(G)} (d_i+d_j))^{\frac{1}{2}} \leq \left( \sum_{v_i v_j \in E(G)} (d_i+d_j)^2 \right)^{\frac{1}{2}} + \sqrt{m}.$$

From the above inequality,

$$m+2 \sum_{v_i v_j \in E(G)} (d_i+d_j) \leq \sum_{v_i v_j \in E(G)} (d_i+d_j)^2 + m+2 \sqrt{m \sum_{v_i v_j \in E(G)} (d_i+d_j)^2}.$$

It is known that,  $\sum_{v_i v_j \in E(G)} (d_i^2 + d_j^2) = \sum_{v_i v_j \in E(G)} ((d_i+d_j)^2 - 2d_i d_j)$ . By expanding the terms under summation,

$$\sum_{v_i v_j \in E(G)} (d_i+d_j)^2 = F(G) + 2R_{-1}^2(G).$$

It is concluded that

$$2 \sum_{v_i v_j \in E(G)} (d_i+d_j) \leq F(G) + 2R_{-1}^2(G) + 2\sqrt{m(F(G) + 2R_{-1}^2(G))}.$$

Hence,

$$4H_{-1}(G) - F(G) - 2R_{-1}^2(G) \leq 2\sqrt{m(F(G) + 2R_{-1}^2(G))}. \quad \square$$

**Theorem 2.12.** Let  $G$  be a connected regular graph with  $m$  edges, then

$$\frac{ABC(G)}{R(G)} \leq \sqrt{2(H_{-1}(G) - m)}.$$

**Proof.** By the definition of ABC index,

$$\sum_{v_i v_j \in E(G)} \sqrt{\frac{d_i + d_j - 2}{d_i d_j}} \geq \sqrt{\sum_{v_i v_j \in E(G)} \frac{d_i + d_j - 2}{d_i d_j}}.$$

It follows that,

$$ABC^2(G) \geq \frac{\sum_{v_i v_j \in E(G)} d_i + d_j - 2}{\sum_{v_i v_j \in E(G)} d_i d_j}.$$

Indeed, it is seen that

$$ABC^2(G) \geq \frac{2H_{-1}(G) - 2m}{R^{-2}(G)}.$$

Hence,

$$\frac{ABC(G)}{R(G)} \geq \sqrt{2(H_{-1}(G) - m)}. \quad \square$$

### 3. Conclusion

Topological indices is the corner stone of the theories in this paper. Therefore, new inequalities and relations are obtained for topological structures throughout this paper. Firstly, the weighted graphs are examined and some special bounds are formed. In continuation, to gain a more intuitive understanding of the topological index of composite graphs and original graphs, some relations are found. Lastly, some relationships are stated between different topological indices.

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