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SOME CHEMICAL INDICES RELATED TO THE NUMBER OF TRIANGLES

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Abstract. Many chemical indices have been invented in theoretical chemistry, such as the Zagreb index, the Lanzhou index, the forgotten index, the Estrada index etc. In this paper, we show that the first Zagreb index is only related to the sum of the number of triangles in a graph and the number of triangles in its complement. Moreover, we determine the sum of the first and second Zagreb index, the Lanzhou index and the forgotten index for a graph and its complement in terms of the number of triangles in a graph and the number of triangles in its complement. Finally, we estimate the Estrada index in terms of order, size, maximum degree and the number of triangles.

1. Introduction

Throughout this paper, we are concerned with connected undirected simple graph only. The *order* of a graph $G = (V, E)$ is $|V(G)| = |V|$ and its *size* is $|E(G)| = |E|$. A *neighbour* of a vertex v is a vertex adjacent to v. The set of all neighbours of v is denoted by $N_G(v)$, or simply by $N(v)$. The *degree* of v is defined to be $d_G(v) = |N_G(v)|$, or simply by d_v. Especially, $\triangle = \triangle(G)$ and $\delta = \delta(G)$ are called as maximum and minimum degree of G, respectively. The *complement* graph $\overline{G}$ of a graph G has the same vertex set $V(G)$, and two vertices are adjacent in $\overline{G}$ if and only if they are not adjacent

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in G. The *first and second Zagreb index* $M_1(G)$ and $M_2(G)$ of a graph G is denoted as

$$M_1(G) = \sum_{u\in V(G)} d_u^2 = \sum_{uv\in E(G)} (d_u + d_v)$$

and

$$M_2(G) = \sum_{uv\in E(G)} d_u d_v.$$

While the *forgotten index* of G is denoted as

$$F(G) = \sum_{u\in V(G)} d_u^3.$$

We notice that $M_1(G)$ and $F(G)$ are defined in a similar way. Indeed, they were defined in the same paper [11], but their fortunes since have been remarkably different. While the First Zagreb index became one of the most popular and well researched topological indices, the other one fell into oblivion and remained there until very recently when it was reintroduced by Furtula and Gutman. Recently Vukičevíc et al. introduced a new topological index for a molecular graph G in [4] named the *Lanzhou index* as

$$Lz(G) = (n-1)M_1(G) - F(G) = \sum_{u\in V(G)} (n-1-d_u)d_u^2 = \sum_{u\in V(G)} \overline{d_u} d_u^2,$$

where d_u and $\overline{d_u}$ denoted the degree of vertex u in G and its complement respectively. Estrada [6] put forward a graph invariant, which was originally referred to as the subgraph centrality but has since become known as the *Estrada index* of a graph G, defined as

$$EE(G) = \sum_{i=1}^{n} e^{\lambda_i},$$

where $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of G. The Estrada index has successfully found applications in various fields, including biochemistry [6], [7] and complex networks [8].

In section 2, we first show that the first Zagreb index is only related to the sum of the number of triangles in a graph and the number of triangles in its complement. Next, we prove that the sum of first and second Zagreb index for a graph and its complement only is depend on the sum of the number of triangles in a graph and the number of triangles in its complement. From another perspective, we present a new method to prove the upper bound and lower bound of the sum of the number of triangles in a graph and the number of triangles in its complement.

In section 3, we apply the results in the previous section to determine the sum of Lanzhou index and forgotten index for a graph and its complement in terms of the number of triangles in a graph and the number of triangles in its complement. Moreover, we also apply the results in the previous

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section to estimate the Estrada index of graphs in terms of order, size, maximum degree, minimum degree and the number of triangles.

2. First and second Zagreb index

Let $|T(G)|$ be the number of triangles and C_n^3 be the number of triples (u, v, w) in G.

Lemma 2.1. *Let G be a graph of order n, and $\overline{G}$ be its complement. Then*

$$\sum_{v \in V(G)} d_v(n-1-d_v) = 2[C_n^3 - (|T(G)| + |T(\overline{G})|)].$$

Proof. On the one hand, the number of triples (u, v, w) where uv is an edge and vw is not an edge is clearly $\sum_{v \in V(G)} d_v(n-1-d_v)$. On the other hand, every set of 3 vertices either contributes 0 to this sum (if either all or none of the 3 edges between them are presented), or contributes 2 (if they have exactly 1 or exactly 2 edges). Therefore, we have

$$\sum_{v \in V(G)} d_v(n-1-d_v) = 2[C_n^3 - (|T(G)| + |T(\overline{G})|)].$$

□

Next, we show that the first Zagreb index is only related to the sum of the number of triangles in a graph and the number of triangles in its complement.

Theorem 2.2. *If G be a graph of order n and size m, then*

$$M_1(G) = 2[(|T(G)| + |T(\overline{G})|) + (n-1)m - C_n^3].$$

Proof. By Lemma 2.1, we have

$$\begin{aligned} 2[C_n^3 - (|T(G)| + |T(\overline{G})|)] &= \sum_{v \in V(G)} d_v(n-1-d_v) \\ &= (n-1)\sum_{v \in V(G)} d_v - \sum_{v \in V(G)} d_v^2 \\ &= 2m(n-1) - M_1(G) \end{aligned}$$

Thus, $M_1(G) = 2[(|T(G)| + |T(\overline{G})|) + (n-1)m - C_n^3]$. □

Theorem 2.3. $M_1(G) + M_1(\overline{G}) = 4(|T(\overline{G})| + |T(G)|) + n(n-1)^2 - 4C_n^3$.

If we only consider that the first Zagreb index for a tree T, then we have the following Corollary 2.4 since $|E(T)| = n-1$.

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Corollary 2.4. $M_1(T) = 2[|T(\overline{T})| + (n-1)^2 - C_n^3]$

By Corollary 2.4, we know that the first Zagreb index for a tree is only depend on the number of triangles in its complement. Goodman [1] estimated the minimum value of $|T(G)|+|T(\overline{G})|$ for a graph G and Lorden [10] derived the exact value.

Theorem 2.5. [10] *Let G be a graph of order n, and $\overline{G}$ be its complement. Then*

$$\min\{|T(G)| + |T(\overline{G})|\} = \begin{cases} \frac{k(k-1)(k-2)}{3} & \text{if } n = 2k, \\ \frac{2k(k-1)(4k+1)}{3} & \text{if } n = 4k+1, \\ \frac{2k(k+1)(4k-1)}{3} & \text{if } n = 4k+3, \end{cases}$$

where k is a nonnegative integer.

Nordhaus-Gaddum-type results are bounds of the sum or the product of a parameter for a graph and its complement. The name Nordhaus-Gaddum-type is given because Nordhaus and Gaddum [9] first initiated this type inequalities on the chromatic number of a graph and its complement in 1956. Since then, Nordhaus-Gaddum-type inequalities for many other graph invariants have been studied in numerous of paper. It is easy to see that the Nordhaus-Goddum-type inequality for the first Zagreb index can be given by the following Theorem 2.6. In fact, Zhang and Baoyindureng have been prove it by the definition of a convex function in [16].

Theorem 2.6. [16] *Let G be a graph of order n, and $\overline{G}$ be its complement. Then*

$$2n(\frac{n-1}{2})^2 \leq M_1(G) + M_1(\overline{G}) \leq n(n-1)^2.$$

The lower bound are obtained on the $\frac{n-1}{2}$-regular graphs and the upper bound are obtained uniquely on K_n.

Bidegreed graph is a graph whose vertices have exactly two degrees $\triangle$ and δ. Das [14] and Hosamani and Basavanagoud [17], independently, proposed a upper bound for the first Zagreb index.

Theorem 2.7. [14, 17] *Let G be a simple graph with order n and size m. Then*

$$M_1(G) \leq 2m(\triangle + \delta) - n\triangle\delta,$$

equality holds if and only if G is regular or bidegreed graphs.

Recall that for a graph with n vertices and m edges, the average value of vertex degrees is $\frac{2m}{n}$. Therefore, $M_1(G) \geq \frac{4m^2}{n}$. Moreover, we have $|T(\overline{G})| + |T(G)| \geq \frac{2m^2}{n} + C_n^3 - m(n-1)$ by Theorem 2.2.

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From another perspective, we present a new method to prove the lower bound of the sum of the number of triangles in a graph and the number of triangles in its complement. By Theorem 2.2 and Theorem 2.7, we have the following Theorem 2.8.

Theorem 2.8. *Let G be a simple graph with order n and size m. Then*

$$\frac{2m^2}{n} + C_n^3 - m(n-1) \le |T(\overline{G})| + |T(G)| \le m(\triangle + \delta + 1 - n) + C_n^3 - \frac{1}{2}n\triangle\delta.$$

The lower bound are obtained on the regular graphs and the upper bound are obtained on regular or bidegreed graphs.

Furthermore, by Theorem 2.3 and Theorem 2.8, we can improve the lower and upper bound for $M_1(G) + M_1(\overline{G})$ in Theorem 2.6.

Corollary 2.9. *Let G be a graph of order n and size m. Then*

$$\frac{8m^2}{n} - 4m(n-1) + n(n-1)^2 \le M_1(G) + M_1(\overline{G}) \le 4m(\triangle + \delta + 1 - n) - 2n\triangle\delta + n(n-1)^2.$$

The lower bound are obtained on the regular graphs and the upper bound are obtained on regular or bidegreed graphs.

From [15], we have

$$M_2(G) + M_2(\overline{G}) = (n - \frac{3}{2})M_1(G) + \frac{n(n-1)^3}{2} - 3m(n-1)^2 + 2m^2.$$

Combining Theorem 2.2, we obtain the following Theorem 2.10.

Theorem 2.10. *Let G be a graph, then we can get that*

$$M_2(G) + M_2(\overline{G}) = (2n-3)[(|T(G)| + |T(\overline{G})|) + (n-1)m - C_n^3] + \frac{n(n-1)^3}{2} - 3m(n-1)^2 + 2m^2.$$

Furthermore, by Theorem 2.8, we get the following Nordhaus-Gaddum-type inequalities for the second Zagreb index.

Corollary 2.11. *Let G be a simple graph with order n and size m. Then*
$(2n-3)[\frac{2m^2}{n} + C_n^3 - m(n-1)] + \frac{n(n-1)^3}{2} - 3m(n-1)^2 + 2m^2 \le M_2(G) + M_2(\overline{G}) \le (2n-3)[(m(\triangle + \delta + 1 - n) + C_n^3 - \frac{1}{2}n\triangle\delta) + (n-1)m - C_n^3] + \frac{n(n-1)^3}{2} - 3m(n-1)^2 + 2m^2$. *The lower bound are obtained on the regular graphs and the upper bound are obtained on regular or bidegreed graphs.*

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3. **Lanzhou and Forgotten and Estrada Index**

We can get several results that can be verified by direct computation by the definition of Nordhaus-Gaddum-type inequalities for Lanzhou index.

Proposition 3.1. *Let K_n, $K_{s,t}$, P_n, S_n and $S_{\frac{n}{2},\frac{n}{2}}$ are complete graph, complete bipartite graph, path, star and balanced double star respectively. Then we have*

(1) $Lz(K_n) + Lz(\overline{K_n}) = 0$.

(2) $Lz(K_{s,t}) + Lz(\overline{K_{s,t}}) = st(n-1)(2n-t-s-2)$.

(3) $Lz(P_n) + Lz(\overline{P}_n) = 2(n^3 - 6n^2 + 13n - 10)$.

(4) $Lz(S_n) + Lz(\overline{S}_n) = n^3 - 4n^2 + 5n - 2$.

(5) $Lz(S_{\frac{n}{2},\frac{n}{2}}) + Lz(\overline{S_{\frac{n}{2},\frac{n}{2}}}) = \frac{1}{2}(3n^3 - 13n^2 + 18n - 2)$.

Next, we show that the Lanzhou index is only related to the sum of the number of triangles in a graph and the number of triangles in its complement.

Theorem 3.2. $Lz(G) + Lz(\overline{G}) = 2(n-1)[C_n^3 - (|T(G)| + |T(\overline{G})|)]$.

Proof. By the definition of Lanzhou index. We have

$$Lz(G) + Lz(\overline{G}) = \sum_{v\in V(G)} (n-1-d_v)d_v^2 + \sum_{v\in V(G)} (n-1-d_v)^2 d_v = (n-1) \sum_{v\in V(G)} (n-1-d_v)d_v.$$

By lemma 2.1, we get $Lz(G) + Lz(\overline{G}) = 2(n-1)[C_n^3 - (|T(G)| + |T(\overline{G})|)]$. □

By the Theorem 2.5, Theorem 2.8, and Theorem 3.2, we have the following Nordhaus-Goddum-type inequality for the Lanzhou index.

Corollary 3.3. *Let G be a graph of order n and size m. Then*

$$n(n-1)\triangle\delta - 2m(n-1)(\triangle + \delta + 1 - n) \leq Lz(G) + Lz(\overline{G}) \leq 2m(n-1)(n-1-\frac{2m}{n}).$$

The lower bound are obtained on regular or bidegreed graphs and the upper bound are obtained on the regular graphs.

Recall that $Lz(G) = (n-1)M_1(G) - F(G)$. Combining the Theorem 2.3 and Theorem 3.2, we obtain the following Theorem 3.4

Theorem 3.4. *Let G be a graph of order n, and $\overline{G}$ be its complement. Then*

$$F(G) + F(\overline{G}) = 6(n-1)(|T(G)| + |T(\overline{G})|) + n(n-1)^2.$$

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By the Theorem 2.5, Theorem 2.8 and Theorem 3.4, we have the following Nordhaus-Goddum-type inequality for the Forgotten index.

Corollary 3.5. *Let G be a graph of order n, and size m. Then*

$$\frac{12m^2}{n}(n-1)+(n^2-6m-n)(n-1)^2 \leq F(G)+F(\overline{G}) \leq 6(n-1)[m(\triangle+\delta+1-n)+C_n^3-\frac{1}{2}n\triangle\delta]+n(n-1)^2.$$

The lower bound are obtained on the regular graphs and the upper bound are obtained regular or bidegreed graphs.

A *walk* W of length k starting at a vertex v and ending at a vertex v_k in G is a sequence of vertices, i.e., $v_0, v_1, v_2, \ldots, v_k$, in which v_i is adjacent to v_{i+1} for each $i = 0, 1, \ldots, k-1$. In particular, if the vertices $v_0, v_1, v_2, \ldots, v_k$ (except the possible v_0 and v_k) are pairwise distinct, then W is well known as a path, and if $v_0 = v_k$, then W is called a *closed walk* . It is well known that the number of closed walks of length k in G is exactly the trace of $A(G)^k$ which, in turn, is the sum of the k th power of the eigenvalues of G (known as the kth spectral moment of G). This fact is of importance in the theory of total π-electron energy, for details see [12], [13] and the references cited therein.

Given a graph G and a vertex v, let $\mathcal{W}_k(G,v)$ and $\mathcal{CW}_k(G,v)$ denote the set of walks and closed walks of length k starting at v in G, and let $W_k(G,v) = |\mathcal{W}_k(G,v)|$ and $CW_k(G,v) = |\mathcal{CW}_k(G,v)|$. Chen and Qian [18] using graph-theoretical techniques, established an inequality regarding the number of walks and closed walks in a graph. Furthermore, they also given an upper bound for the Estrada index.

Theorem 3.6. [18] *Let G be a graph with order n and size m. Then*

$$W_k(G) \leq M_1(G)\triangle^{k-2}, \ for\ any\ k \geq 3, \ (1)$$

$$W_k(G) \leq 2M_2(G)\triangle^{k-3}, \ for\ any\ k \geq 4, \ (2)$$

$$CW_k(G) \leq M_1(G)\triangle^{k-3}, \ for\ any\ k \geq 3, \ (3)$$

$$CW_k(G) \leq 2M_2(G)\triangle^{k-4}, \ for\ any\ k \geq 4, \ (4)$$

$$EE(G) < n+m+\frac{M_1(G)}{\triangle^3}(e^{\triangle}-1-\triangle-\frac{\triangle^2}{2}),$$

$$EE(G) < n+m+|T(G)|+\frac{2M_1(G)}{\triangle^4}(e^{\triangle}-1-\triangle-\frac{\triangle^2}{2}-\frac{\triangle^3}{6}).$$

The equalities holds in (1)-(2) *if and only if G is regular; the equalities holds in* (3)-(4) *if and only if k is even and each component of G is the complete bipartite graph $K_{\triangle,\triangle}$.*

Next, we apply the results in the section 2 to estimate the Estrada index, the number of walks and closed walks in terms of order, size, maximum degree and triangles. And the following Lemma 3.7 will be used.

Lemma 3.7. [14] *Let G be a graph with order n and size m. Then*

$$M_2(G) \leq 2m^2 - (n-1)m\delta + \frac{1}{2}(\delta - 1)M_1(G).$$

By using the Theorem 2.7, Theorem 3.6 and Lemma 3.7, we have the following results.

Theorem 3.8. *Let G be a graph with order n and size m. Then*

$$W_k(G) \leq (2m(\triangle + \delta) - n \triangle \delta)\triangle^{k-2}, \ for\ any\ k \geq 3,$$

$$W_k(G) \leq [4m^2 - 2(n-1)m\delta + (\delta - 1)(2m(\triangle + \delta) - n \triangle \delta)]\triangle^{k-3}, \ for\ any\ k \geq 4,$$

$$CW_k(G) < [2m(\triangle + \delta) - n \triangle \delta]\triangle^{k-3}, \ for\ any\ k \geq 3,$$

$$CW_k(G) < [4m^2 - 2(n-1)m\delta + (\delta - 1)(2m(\triangle + \delta) - n \triangle \delta)]\triangle^{k-4}, \ for\ any\ k \geq 4,$$

$$EE(G) < n + m + \frac{2m(\triangle + \delta) - n \triangle \delta}{\triangle^3}(e^{\triangle} - 1 - \triangle - \frac{\triangle^2}{2}),$$

$$EE(G) < n + m + |T(G)| + \frac{4m^2 - 2(n-1)m\delta + (\delta - 1)[2m(\triangle + \delta) - n \triangle \delta]}{\triangle^4}(e^{\triangle} - 1 - \triangle - \frac{\triangle^2}{2} - \frac{\triangle^3}{6}).$$

The equalities holds in (1) *if and only if G is regular; the equalities holds in* (2) *if and only if G is complete graph.*

Zhou and Du [16] establish lower bounds for the Estrada index by using the first Zagreb index.

Theorem 3.9. [16] *Let G be a graph with order n and size m. Then*

$$EE(G) \geq n + m + |T(G)| + (e + e^{-1})[M_1(G) - m] + 15(e - e^{-1} - \frac{7}{3})|T(G)|,$$

with either equality if and only if G consists of m copies of complete graph on two vertices and possibly isolated vertices.

By using the Theorem 2.7 and Theorem 3.9, we have the following results.

Theorem 3.10. *Let G be a graph with order n and size m. Then*

$$EE(G) \geq n + m + |T(G)| + (e + e^{-1})[2(|T(G)| + |T(\overline{G})| - C_n^3) + (2n-3)m] + 15(e - e^{-1} - \frac{7}{3})|T(G)|,$$

with either equality if and only if G consists of m copies of complete graph on two vertices and possibly isolated vertices.

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