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Some Relations and Bounds for the General First Zagreb Index

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Abstract

We obtain some relations and sharp bounds for the general first Zagreb index. Also, we provide some linear recurrence relations with constant coefficients for the sequence of the general first Zagreb indices which are modifications of a result appeared in [L. Bedratyuk, O. Savenko, The star sequence and the general first Zagreb index, MATCH Commun. Math. Comput. Chem. 79 (2018) 407-414]. Moreover, we show that by using the Stirling numbers of the first kind, for each integer $p \geq \Delta(G)$, the general first Zagreb index $Z_p(G)$ can be expressed as a linear combination of $Z_0(G)$, $Z_1(G)$, ..., $Z_{\Delta-1}(G)$.

1 Introduction

Let G be a simple graph (without isolated vertex) with vertex set $V(G)$ and edge set $E(G)$ such that $|V(G)| = n$ and $|E(G)| = m$. Two vertices of G which are connected by an edge are called adjacent and the number of vertices adjacent to a given vertex $v \in V(G)$ is the degree of v and is denoted by $\deg(v)$. In [13] and [14] Li et al. considered the general first Zagreb index of a graph G as

$$Z_p(G) = \sum_{uv \in E(G)} \left(\deg(u)^{p-1} + \deg(v)^{p-1}\right) = \sum_{u \in V(G)} \deg(u)^p$$

in which p is a real number. Specially, we see that $Z_0(G) = n$, $Z_1(G) = 2m$, $Z_2(G) = M_1(G)$ which is the first Zagreb index and $Z_3(G) = F(G)$ which is known as the forgotten topological index, see [1–5, 9, 12, 15, 16] for more details.

In [7] some combinatorial identities, relating $Z_p(G)$ with counts of various subgraphs contained in the graph G are presented. The Stirling number of the first kind, denoted by $s(n,k)$, is defined by the rule that $(-1)^{n-k}s(n,k)$ is the number of permutations of $\{1,2,...,n\}$ with k cycles, and the Stirling number $S(n,k)$ of the second kind counts the number of ways to partition a set of n elements into k nonempty subsets, see [8] for more details. Gutman et. al. in [10] and [11], among some other nice results, obtained the following result which is a generalized form of the Goubko's theorem.

Theorem 1. *Let G be a connected graph with n vertices, m edges and n_1 pendant vertices. Then $M_1(G) \geq 16m - 16n + 9n_1$ and the equality holds if and only if all non-pendant vertices of G are of degree 4.*

We use their method applied for the proof of this theorem to obtail some other relations and bounds for the general first Zagreb index. Also, it is shown in [6] that

$$Z_p(G) = 2S_1(G) + \sum_{i=2}^{p} i!S(p,i)S_i(G)$$

in which $p \geq 1$ and $S_i(G)$ is the number of subgraphs of G that are isomorphic to the star $S_i = K_{1,i}$. Moreover, in [6] by using the ordinary generating function for the integer sequence $\{Z_p(G)\}_{p\geq 0}$, i.e.

$$\sum_{p=0}^{\infty} Z_p(G)t^p = \frac{\sum_{k=0}^{n-1}\left(\sum_{i=0}^{k} s(n+1,n+1-(k-i))\ Z_i(G)\right)\ t^k}{(1-t)(1-2t)\cdots(1-nt)}$$

it is deduced that

$$Z_p(G) + \sum_{i=1}^{n} s(p+1,p+1-i)\ Z_{p-i}(G) = 0, \quad p \geq n.$$

This is a linear recurrence relation of order n (the number of vertices of G) for the sequence of the general first Zagreb indices. This relation shows that for each integer $p \geq n$ we can express $Z_p(G)$ as a linear combinatin of n previous general first Zagreb indices $Z_{p-1}(G)$, $Z_{p-2}(G)$, ..., $Z_{p-n}(G)$.

In this paper, we give some modifications of these results and among some other resulats, we specially show that (see Theorem 5 and Corollary 7)

$$\sum_{i=1}^{p+1} s(p+1,i)\ Z_{i-1}(G) = 0, \quad p \geq \Delta(G),$$

$$\sum_{i=1}^{\ell+1} s(\ell+1,i)\ Z_{i-1}(G) = \sum_{k\geq\ell} \frac{k!}{(k-\ell)!}\ n_{k+1}, \quad \ell \geq 1,$$

$$Z_p(G)=\sum_{i=1}^{\Delta}\left[\sum_{j=1}^{p-\Delta+1}\ \sum_{\Delta+1\leq x_1<x_2<\cdots<x_j=p+1}(-1)^j s(x_j,x_{j-1})s(x_{j-1},x_{j-2})\cdots s(x_2,x_1)s(x_1,i)\right]Z_{i-1}(G).$$

2 Main results

For each integer $k \geq 1$ denote the number of vertices of degree k in G by n_k. Specially, n_1 is the number of pendant vertices. Therefore,

$$\sum_{k\geq 1} n_k = n, \quad \sum_{k\geq 1} kn_k = 2m, \quad \sum_{k\geq 1} k^2 n_k = M_1(G), \quad \sum_{k\geq 1} k^3 n_k = F(G),$$

and

$$\sum_{k\geq 1} k^p n_k = Z_p(G), \quad p \in \mathbb{R}.$$

Theorem 2. *Let G be an n-vertex graph of size m. Then,*

i) $M_1(G) \geq 18m - 20n + 12n_1 + 6n_2 + 2n_3$ *with equality just when* $\Delta(G) \leq 5$,

ii) $M_1(G) \geq 16m - 15n + 8n_1 + 3n_2 - n_4$ *with equality just when* $\Delta(G) \leq 5$,

iii) $M_1(G) \geq 16m - 16n + 9n_1 + 4n_2 + n_3$ *with equality just when* $\Delta(G) \leq 4$,

iv) $M_1(G) \geq 14m - 12n + 6n_1 + 2n_2$ *with equality just when* $\Delta(G) \leq 4$,

v) $M_1(G) \geq 12m - 8n + 3n_1 - n_3$ *with equality just when* $\Delta(G) \leq 4$,

vi) $M_1(G) \geq 12m - 9n + 4n_1 + n_2$ *with equality just when* $\Delta(G) \leq 3$.

vii) $M_1(G) \geq 10m - 6n + 2n_1$ *with equality just when* $\Delta(G) \leq 3$,

viii) $M_1(G) \geq 8m - 4n + n_1$ *with equality just when* $\Delta(G) \leq 2$,

ix) $M_1(G) \geq 6m - 2n$ *with equality just when* $\Delta(G) \leq 2$,

Proof. For each pair of real numbers a, b we have

$$\sum_{k\geq 1}(k-a)(k-b)n_k = \sum_{k\geq 1}(k^2-(a+b)k+ab)n_k = M_1(G) - 2m(a+b) + abn.$$

Hence,

$$M_1(G) = 2m(a+b) - abn + \sum_{k\geq 1}(k-a)(k-b)n_k.$$

Now with the assumption $a = 4,\ b = 5$ we see that

$$\begin{aligned} M_1(G) &= 18m - 20n + \sum_{k\geq 1}(k-4)(k-5)n_k \\ &= 18m - 20n + 12n_1 + 6n_2 + 2n_3 + \sum_{k\geq 6}(k-4)(k-5)n_k \\ &\geq 18m - 20n + 12n_1 + 6n_2 + 2n_3. \end{aligned}$$

Obviously in the last relation, the equality holds if and only if $\Delta(G) < 6$. Similarly, for the cases (ii) to (ix) let (a,b) be $(3,5)$, $(4,4)$, $(3,4)$, $(2,4)$, $(3,3)$, $(2,3)$, $(2,2)$ and $(1,2)$, respectively. ■

Corollary 1. *If* $\Delta(G) \leq 5$*, then*

$$n_4 = 5n - 2m - 4n_1 - 3n_2 - 2n_3, \quad n_5 = 2m - 4n + 3n_1 + 2n_2 + n_3.$$

Proof. by Theorem 2 parts (i) and (ii) we have

$$18m - 20n + 12n_1 + 6n_2 + 2n_3 = M_1(G) = 16m - 15n + 8n_1 + 3n_2 - n_4.$$

This implies that $n_4 = 5n - 2m - 4n_1 - 3n_2 - 2n_3$. Now we have

$$\begin{aligned} n_5 &= n - n_1 - n_2 - n_3 - n_4 \\ &= n - n_1 - n_2 - n_3 - (5n - 2m - 4n_1 - 3n_2 - 2n_3) \\ &= 2m - 4n + 3n_1 + 2n_2 + n_3. \end{aligned}$$

■

Similarly, by comparing part (iii) with (iv), and part (vi) with (vii) in Theorem 2 we can obtain the following two results, respectively.

Corollary 2. *If G is a molecular graph (i.e.* $\Delta(G) \leq 4$*), then*

$$n_3 = 4n - 2m - 3n_1 - 2n_2, \quad n_4 = 2m - 3n + 2n_1 + n_2.$$

Corollary 3. *If* $\Delta(G) \leq 3$*, then*

$$n_2 = 3n - 2m - 2n_1, \quad n_3 = 2m - 2n + n_1.$$

Theorem 3. *For each n-vertex graph G of size m we have*

i) $F(G) \geq 12M_1(G) - 94m + 60n - 24n_1 - 6n_2$ *with equality just when* $\Delta(G) \leq 5$.

ii) $F(G) \geq 9M_1(G) - 52m + 24n - 6n_1$ *and the equality holds if and only if G is a molecular graph, i.e.* $\Delta(G) \leq 4$.

iii) $F(G) \geq 6(M_1(G) + n) - 22m$ *with equality just when* $\Delta(G) \leq 3$.

Proof. Note that for real numbers a, b, c we have

$$\sum_{k\geq 1}(k-a)(k-b)(k-c)n_k = F(G) - (a+b+c)M_1(G) + 2(ab+ac+bc)m - abcn,$$

which implies that

$$F(G) = (a+b+c)M_1(G) - 2(ab+ac+bc)m + abcn + \sum_{k\geq 1}(k-a)(k-b)(k-c)n_k.$$

Now, if we let $a = 3,\ b = 4,\ c = 5$, then we have

$$\begin{aligned} F(G) &= 12M_1(G) - 94m + 60n + \sum_{k\geq 1}(k-3)(k-4)(k-5)n_k \\ &= 12M_1(G) - 94m + 60n - 24n_1 - 6n_2 + \sum_{k\geq 6}(k-3)(k-4)(k-5)n_k, \end{aligned}$$

and (i) follows directly from it.

For the case (ii) it is sufficient to let $a = 2,\ b = 3,\ c = 4$ and for (iii) let $a = 1,\ b = 2,\ c = 3$. ■

Corollary 4. *If G is a molecular graph (i.e. $\Delta(G) \leq 4$), then*

$$M_1(G) = 14m - 12n + 6n_1 + 2n_2$$

and hence,

$$14m - 12n \leq M_1(G) \leq 14m - 4n.$$

Proof. By Theorem 3 parts (i) and (ii) we see that

$$9M_1(G) - 52m + 24n - 6n_1 = F(G) = 12M_1(G) - 94m + 60n - 24n_1 - 6n_2.$$

Now the results follow because $0 \leq n_i \leq n$ for $i \in \{1, 2\}$. ■

Corollary 5. *If $\Delta(G) \leq 3$, then* $M_1(G) = 10m - 6n + 2n_1$.

Theorem 4. *For each n-vertex graph G of size m we have*

$$Z_4(G) \geq 10F(G) - 35M_1(G) + 100m - 24n.$$

The equality holds if and only if G is a molecular graph, i.e. $\Delta(G) \leq 4$.

Proof. By considering the relation

$$\begin{aligned}\sum_{k\geq 1}(k-1)(k-2)(k-3)(k-4)n_k &= \sum_{k\geq 1}(k^4 - 10k^3 + 35k^2 - 50k + 24)n_k \\ &= Z_4(G) - 10F(G) + 35M_1(G) - 100m + 24n,\end{aligned}$$

the result follows directly. ■

By using this method and by choosing other suitable values for $a, b, c, d, ...$ we can obtain many different relations and bounds for the general first Zagreb indices. We drop it here but we want to consider another general case as below.

For each integer $\ell \geq 1$ let $(x)_\ell = x(x-1)(x-2)\cdots(x-(\ell-1))$. The following result is well known (for example see Proposition 5.3.3 in [8]).

Lemma 1. $(x)_\ell = \sum_{i=1}^{\ell} s(\ell, i)x^i$.

The following result provides a linear recurrence relation with constant coefficients for the sequence of the general first Zagreb indices.

Theorem 5. *Let G be a graph (which has no isolated vertex). Then, for each integer $\ell \geq 1$ we have*

$$\sum_{i=1}^{\ell+1} s(\ell+1, i)\ Z_{i-1}(G) = \sum_{k\geq \ell} \frac{k!}{(k-\ell)!}\ n_{k+1}$$

Proof. For each integer $\ell \geq 1$, from Lemma 1, we can easily see that

$$(x-1)(x-2)\cdots(x-\ell) = \sum_{i=1}^{\ell+1} s(\ell+1, i)\ x^{i-1}.$$

Therefore,

$$\begin{aligned}\sum_{i=1}^{\ell+1} s(\ell+1,i)\ Z_{i-1}(G) &= \sum_{i=1}^{\ell+1}\left(s(\ell+1,i)\sum_{k\geq 1} k^{i-1}n_k\right)\\ &= \sum_{i=1}^{\ell+1}\sum_{k\geq 1} s(\ell+1,i)\ k^{i-1}n_k\\ &= \sum_{k\geq 1}\left(\sum_{i=1}^{\ell+1} s(\ell+1,i)\ k^{i-1}\right) n_k\\ &= \sum_{k\geq 1}\Big((k-1)(k-2)\cdots(k-\ell)\Big)n_k\\ &= \sum_{k\geq \ell}\frac{k!}{(k-\ell)!}\ n_{k+1}.\end{aligned}$$

■

By considering the special cases $\ell = 1$, $\ell = 2$ and $\ell = 3$ in Theorem 5 we obtain the following result.

Corollary 6. *If G is a graph with n vertices and m edges, then*

i) $\sum_{k\geq 1} k\ n_{k+1} = 2m - n$,

ii) $\sum_{k\geq 2} k(k-1)\ n_{k+1} = 2n - 6m + M_1(G)$,

iii) $\sum_{k\geq 3} k(k-1)(k-2)\ n_{k+1} = F(G) - 6M_1(G) + 22m - 6n$.

Note that if $\Delta(G) \leq 3$, then part (iii) of Corollay 6 implies that $0 = F(G)-6M_1(G)+22m-6n$ which coincides with part (iii) of Theorem 3. Since $n_k = 0$ for each $k \geq 1+\Delta(G)$, using Theorem 5 the following result directly follows.

Corollary 7. *For each integer $p \geq \Delta(G)$ we have*

$$\sum_{i=1}^{p+1} s(p+1,i)\ Z_{i-1}(G) = 0.$$

Specially,

$$Z_p(G) = -\sum_{i=1}^{p} s(p+1,i)\ Z_{i-1}(G).$$

For example, when $\Delta(G) = 3$ then using the facts $s(4,1) = -6$, $s(4,2) = 11$, $s(4,3) = -6$, $s(4,4) = 1$ and by inserting $p = 3$ we can write $Z_3(G)-6M_1(G)+22m-6n = 0$, which confirms part (iii) of Theorem 3, and similarly when $\Delta = 4$ then (with $p = 4$) we have $Z_4(G) - 10Z_3(G) + 35M_1(G) - 100m + 24n = 0$ which confirms Theorem 4. Note that by Corollary 7 (with $p = \Delta + 1$) and by using the Stirling numbers of the first kind, $Z_{\Delta+1}(G)$ can be expressed as a linear combination of $Z_0(G)$, $Z_1(G)$, ..., $Z_\Delta(G)$. Since $Z_\Delta(G)$, with $p = \Delta$ in Corollary 7, can also be expressed as a linear combination of $Z_0(G)$, $Z_1(G)$, ..., $Z_{\Delta-1}(G)$, it is possible to express $Z_{\Delta+1}(G)$ as a linear combination of $Z_0(G)$, $Z_1(G)$, ..., $Z_{\Delta-1}(G)$. Inductively, this can be done for each $Z_p(G)$ with $p \geq \Delta$.

Theorem 6. *Let G be graph with the maximum degree Δ. Then, for each integer $p \geq \Delta$ we have*

$$Z_p(G) = \sum_{i=1}^{\Delta} \left[\sum_{j=1}^{p-\Delta+1} \sum_{\Delta+1 \leq x_1 < x_2 < \cdots < x_j = p+1} (-1)^j s(x_j, x_{j-1}) s(x_{j-1}, x_{j-2}) \cdots s(x_2, x_1) s(x_1, i) \right] Z_{i-1}(G)$$

Proof. We proceed by induction on p. For the base case $p = \Delta$, by using Corollary 7, we have

$$\begin{aligned} Z_\Delta(G) &= \sum_{i=1}^{\Delta} \Big[- s(\Delta+1, i) \Big] Z_{i-1}(G) \\ &= \sum_{i=1}^{\Delta} \left[\sum_{j=1}^{\Delta-\Delta+1} \sum_{\Delta+1 \leq x_1 = \Delta+1} (-1)^j s(x_1, i) \right] Z_{i-1}(G). \end{aligned}$$

Also, for $p = \Delta + 1$ by Corollary 7 we see that

$$\begin{aligned} Z_{\Delta+1}(G) &= \left(- \sum_{i=1}^{\Delta} s(\Delta+2, i)\ Z_{i-1} \right) - s(\Delta+2, \Delta+1)\ Z_\Delta(G) \\ &= \sum_{i=1}^{\Delta} \Big[- s(\Delta+2, i) + s(\Delta+2, \Delta+1) s(\Delta+1, i) \Big] Z_{i-1}(G) \\ &= \sum_{i=1}^{\Delta} \left[\sum_{j=1}^{\Delta+1-\Delta+1} \sum_{\Delta+1 \leq x_1 < \cdots < x_j = \Delta+2} (-1)^j s(x_j, x_{j-1}) \cdots s(x_1, i) \right] Z_{i-1}(G). \end{aligned}$$

Now assume that the statement holds for each integer p' with $\Delta \leq p' < p$ and we want to show that it holds for p. By Corollary 7 we have

$$\begin{aligned} Z_p(G) &= - \sum_{i=1}^{p} s(p+1, i)\ Z_{i-1}(G) \\ &= - \sum_{i=1}^{\Delta} s(p+1, i)\ Z_{i-1}(G) - \sum_{i=\Delta+1}^{p} s(p+1, i)\ Z_{i-1}(G) \\ &= - \sum_{i=1}^{\Delta} s(p+1, i)\ Z_{i-1}(G) - \sum_{k=\Delta+1}^{p} s(p+1, k)\ Z_{k-1}(G) \end{aligned}$$

The induction hypothesis implies that

$$Z_{k-1}(G) = \sum_{i=1}^{\Delta} \left(\sum_{j=1}^{k-\Delta} \sum_{\Delta+1 \leq x_1 < \cdots < x_j = k} (-1)^j s(x_j, x_{j-1}) \cdots s(x_1, i) \right) Z_{i-1}(G)$$

Therefore,

$$\begin{aligned} Z_p(G) &= \sum_{i=1}^{\Delta} \Bigg[- s(p+1, i) \\ &\quad - \sum_{k=\Delta+1}^{p} \sum_{j=1}^{k-\Delta} \sum_{\Delta+1 \leq x_1 < \cdots < x_j = k} (-1)^j s(p+1, k) s(x_j, x_{j-1}) \cdots s(x_1, i) \Bigg] Z_{i-1}(G) \\ &= \sum_{i=1}^{\Delta} \Bigg[- s(p+1, i) \\ &\quad + \sum_{k=\Delta+1}^{p} \sum_{j=1}^{k-\Delta} \sum_{\Delta+1 \leq x_1 < \cdots < x_j = k} (-1)^{j+1} s(p+1, x_j) s(x_j, x_{j-1}) \cdots s(x_1, i) \Bigg] Z_{i-1}(G) \\ &= \sum_{i=1}^{\Delta} \Bigg[- s(p+1, i) \\ &\quad + \sum_{j=1}^{p-\Delta} \sum_{\Delta+1 \leq x_1 < \cdots < x_{j+1} = p+1} (-1)^{j+1} s(x_{j+1}, x_j) s(x_j, x_{j-1}) \cdots s(x_1, i) \Bigg] Z_{i-1}(G) \\ &= \sum_{i=1}^{\Delta} \Bigg[- s(p+1, i) \\ &\quad + \sum_{j'=2}^{p-\Delta+1} \sum_{\Delta+1 \leq x_1 < \cdots < x_{j'} = p+1} (-1)^{j'} s(x_{j'}, x_{j'-1}) s(x_{j'-1}, x_{j'-2}) \cdots s(x_1, i) \Bigg] Z_{i-1}(G) \\ &= \sum_{i=1}^{\Delta} \Bigg[\sum_{j'=1}^{p-\Delta+1} \sum_{\Delta+1 \leq x_1 < \cdots < x_{j'} = p+1} (-1)^{j'} s(x_{j'}, x_{j'-1}) s(x_{j'-1}, x_{j'-2}) \cdots s(x_1, i) \Bigg] Z_{i-1}(G). \end{aligned}$$

■

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