Kragujevac Journal of Mathematics
Volume 38(1) (2014), Pages 95–103.

COUNTING RELATIONS FOR GENERAL ZAGREB INDICES

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Abstract. The first and second general Zagreb indices of a graph G, with vertex set V and edge set E, are defined as $M_1^k = \sum_{v\in V} d(u)^k$ and $M_2^k = \sum_{uv\in E} [d(u)\, d(v)]^k$, where $d(v)$ is the degree of the vertex v of G. We present combinatorial identities, relating M_1^k and M_2^k with counts of various subgraphs contained in the graph G.

1. Introduction

Throughout this paper we consider finite undirected and simple graphs. Let G be such a graph, with vertex set $V = V(G)$ and edge set $E = E(G)$. Thus, G has $|V|$ vertices and $|E|$ edges. The degree (= number of first neighbors) of a vertex $u \in V(G)$ is denoted by $d_G(u)$ or simply by $d(u)$ when the underlying graph is evident. For $u, v \in V(G)$, the distance (= length of a shortest path) between u and v is denoted by $d(u, v)$. The diameter of the graph G is the greatest distance between its two vertices, and is denoted by $\mathrm{diam}(G)$.

In what follows, the path, star, and cycle with n vertices will be denoted by P_n, $K_{1,n-1}$, and C_n respectively.

Let G and H be graphs. We denote by $\sigma_G(H)$ the number of distinct subgraphs of the graph G which are isomorphic to H. In particular, the graph G has $\sigma_G(P_1)$ vertices, $\sigma_G(P_2)$ edges, and $\sigma_G(C_3)$ triangles. In addition,

$$\sigma_G(K_{1,m}) = \sum_{v\in V(G)} \binom{d(v)}{m}. \tag{1.1}$$

Let α and β be positive integers. The double star $D_{\alpha,\beta}$ is the tree on $\alpha + \beta + 2$ vertices, obtained from the path P_2, by attaching α pendent vertices to its one vertex, and β pendent vertices to its other vertex.

Key words and phrases. Degree (of vertex), Zagreb index, General Zagreb index.
2010 *Mathematics Subject Classification.* Primary: 05C07, Secondary: 05C90.
Received: April 21, 2014.

It is easy to see that for $\alpha \neq \beta$,

$$\sigma_G(D_{\alpha,\beta}) = \sum_{uv\in E(G)} \left[\binom{d(u)-1}{\alpha}\binom{d(v)-1}{\beta} + \binom{d(u)-1}{\beta}\binom{d(v)-1}{\alpha}\right] \tag{1.2}$$

whereas

$$\sigma_G(D_{\alpha,\alpha}) = \sum_{uv\in E(G)} \binom{d(u)-1}{\alpha}\binom{d(v)-1}{\alpha}. \tag{1.3}$$

2. Zagreb and general Zagreb indices

In the 1970s, Trinajstić and one of the present authors introduced two vertex–degree–based graph invariants [18, 17], that eventually were named the first and the second Zagreb indices [1]. These are defined as

$$M_1(G) = \sum_{v\in V(G)} d(v)^2$$

and

$$M_2(G) = \sum_{uv\in E(G)} d(u)\,d(v).$$

The first Zagreb index satisfies the important identity

$$M_1(G) = \sum_{uv\in E(G)} [d(u)+d(v)]$$

which was recognized in the mathematico–chemical literature only around 2010 [8]. Notice that this relation is the special case of Eq. (2.1) for $n = 1$, which in turn is a special case of the recently discovered formula (2.2) for $f(v) := d(v)^{n+1}$ [9]

$$\sum_{v\in V(G)} d(v)^{n+1} = \sum_{uv\in E(G)} \left[d(u)^n + d(v)^n\right] \tag{2.1}$$

$$\sum_{v\in V(G)} f(v) = \sum_{uv\in E(G)} \left[\frac{f(u)}{d(u)} + \frac{f(v)}{d(v)}\right]. \tag{2.2}$$

In [21], Li and Zheng introduced the first general Zagreb index as

$$M_1^k(G) = \sum_{v\in V(G)} d(v)^k \tag{2.3}$$

where $k \in \mathbb{R}$. Obviously $M_1^0(G) = |V|$, $M_1^1(G) = 2|E|$, and $M_1^2(G) \equiv M_1(G)$. It is worth noting that a term identical to $M_1^3(G)$ was considered already in [18].

In analogy with Eq. (2.3), we now define the second general Zagreb index as

$$M_2^k(G) = \sum_{uv\in E(G)} [d(u)\,d(v)]^k \tag{2.4}$$

where $k \in \mathbb{R}$. Obviously $M_2^0(G) = |E|$ and $M_2^1(G) \equiv M_2(G)$.

In 1992, Székely, Clark, and Entringer [26] proved that for every integer $k \geq 1$, $M_1^k(G) \leq [M_1^{1/k}(G)]^k$. De Caen [7] proved that for every simple graph G $M_1(G) \leq |V| \left(\frac{2|E|}{|V|-1} + |V| - 2\right)$. This bound was generalized to hypergraphs by Bey [2] and sharpened by Das [4, 5]. De Caen's inequality was also used by Li and Pan[20] to provide an upper bound on the largest eigenvalue of the Laplacian of a graph.

In [3], Cioaba proved that for any positive number k,

$$M_1^{k+1}(G) \leq \frac{2|E|}{|V|}\Big[M_1^k(G) + (|V|-1)(\Delta^k - \delta^k)\Big] - \frac{\Delta^k - \delta^k}{|V|} M_1(G)$$

where Δ and δ are, respectively, the maximum and minimum degrees of the graph G.

Surveys on Zagreb indices are found in [25, 14, 6, 12, 16, 13]. In [29, 28, 22] various properties and relations of the first general Zagreb index are discussed. In addition to this, Edelberg et al. [11] elaborated the concept of subtree counting, using the characteristic polynomial of the distance matrix of a tree. Motivated by these results, we have proved a few combinatorial counting identities pertaining to the first and second general Zagreb indices.

3. Main Results

Theorem 3.1. *Let G be a simple graph. Then*

$$M_1^2(G) = 2\,\sigma_G(K_{1,2}) + 2\,|E| \tag{3.1}$$

$$M_1^3(G) = 3!\,\sigma_G(K_{1,3}) + 6\,\sigma_G(K_{1,2}) + 2\,|E| \tag{3.2}$$

$$M_1^4(G) = 4!\,\sigma_G(K_{1,4}) + 36\,\sigma_G(K_{1,3}) + 14\,\sigma_G(K_{1,2}) + 2\,|E| \tag{3.3}$$

$$\begin{aligned}
M_1^5(G) &= 5!\,\sigma_G(K_{1,5}) + 240\,\sigma_G(K_{1,4}) + 150\,\sigma_G(K_{1,3}) \\
&\quad + 30\,\sigma_G(K_{1,2}) + 2\,|E| \\
M_1^6(G) &= 6!\,\sigma_G(K_{1,6}) + 1800\,\sigma_G(K_{1,5}) + 1560\,\sigma_G(K_{1,4}) \\
&\quad + 540\,\sigma_G(K_{1,3}) + 62\,\sigma_G(K_{1,2}) + 2\,|E| \\
M_1^7(G) &= 7!\,\sigma_G(K_{1,7}) + 15120\,\sigma_G(K_{1,6}) + 16800\,\sigma_G(K_{1,5}) \\
&\quad + 8400\,\sigma_G(K_{1,4}) + 1806\,\sigma_G(K_{1,3}) + 126\,\sigma_G(K_{1,2}) + 2\,|E| \\
M_1^8(G) &= 8!\,\sigma_G(K_{1,8}) + 141120\,\sigma_G(K_{1,7}) + 191520\,\sigma_G(K_{1,6}) \\
&\quad + 126000\,\sigma_G(K_{1,5}) + 40824\,\sigma_G(K_{1,4}) + 5796\,\sigma_G(K_{1,3}) \\
&\quad + 254\,\sigma_G(K_{1,2}) + 2\,|E| \\
M_1^9(G) &= 9!\,\sigma_G(K_{1,9}) + 1451520\,\sigma_G(K_{1,8}) + 2328480\,\sigma_G(K_{1,7}) \\
&\quad + 1905120\,\sigma_G(K_{1,6}) + 834120\,\sigma_G(K_{1,5}) + 186480\,\sigma_G(K_{1,4}) \\
&\quad + 10150\,\sigma_G(K_{1,3}) + 510\,\sigma_G(K_{1,2}) + 2\,|E|
\end{aligned}$$

$$\begin{aligned} M_1^{10}(G) = {} & 10!\,\sigma_G(K_{1,10}) + 16329600\,\sigma_G(K_{1,9}) + 30240000\,\sigma_G(K_{1,8}) \\ & + 29635200\,\sigma_G(K_{1,7}) + 16435440\,\sigma_G(K_{1,6}) \\ & + 5103000\,\sigma_G(K_{1,5}) + 818520\,\sigma_G(K_{1,4}) + 55980\,\sigma_G(K_{1,3}) \\ & + 1022\,\sigma_G(K_{1,2}) + 2\,|E|. \end{aligned}$$

Proof. Eq. (3.1) is a well known relation for the ordinary first Zagreb index [13]. The other equalities in Theorem 3.1 are obtained by consecutively applying Eqs. (1.1) and (2.3).

In particular, by applying Eqs. (1.1), (2.3), and (3.1) we get

$$\begin{aligned} \sigma_G(K_{1,3}) &= \sum_{v\in V(G)} \binom{d(v)}{3} = \frac{1}{3!} \sum_{v\in V(G)} d(v)[d(v)-1][d(v)-2] \\ &= \frac{1}{3!}\left[\sum_{v\in V(G)} d(v)^3 - 3\sum_{v\in V(G)} d(v)^2 + 2\sum_{v\in V(G)} d(v)\right] \\ &= \frac{1}{3!}\Big[M_1^3(G) - 3\,M_1^2(G) + 2\,M_1^1(G)\Big] \\ &= \frac{1}{3!}\Big[M_1^3(G) - 3\Big(2\,\sigma_G(K_{1,2}) + 2\,|E|\Big) + 2\Big(2\,|E|\Big)\Big] \end{aligned}$$

from which Eq. (3.2) straightforwardly follows. Next, using Eqs. (1.1), (2.3), (3.1), and (3.2), we get

$$\begin{aligned} \sigma_G(K_{1,4}) &= \sum_{v\in V(G)} \binom{d(v)}{4} = \frac{1}{4!} \sum_{v\in V(G)} d(v)[d(v)-1][d(v)-2][d(v)-3] \\ &= \frac{1}{4!}\left[\sum_{v\in V(G)} d(v)^4 - 6\sum_{v\in V(G)} d(v)^3 + 11\sum_{v\in V(G)} d(v)^2 - 6\sum_{v\in V(G)} d(v)\right] \\ &= \frac{1}{4!}\Big[M_1^4(G) - 6\,M_1^3(G) + 11\,M_1^2(G) - 6\,M_1^1(G)\Big] \\ &= \frac{1}{3!}\Big[M_1^3(G) - 6\Big(3!\,\sigma_G(K_{1,3}) + 6\,\sigma_G(K_{1,2}) + 2\,|E|\Big) \\ &\quad + 11\Big(2\,\sigma_G(K_{1,2}) + 2\,|E|\Big) - 6\Big(2\,|E|\Big)\Big] \end{aligned}$$

from which Eq. (3.3) straightforwardly follows. The remaining equalities are obtained recursively in a fully analogous manner. □

Corollary 3.1. *Let G be a simple graph. Then,*

$$\begin{aligned}
M_1^3(G) &= 3!\,\sigma_G(K_{1,3}) + 3\,M_1^2(G) - 4\,|E| \\
M_1^4(G) &= 4!\,\sigma_G(K_{1,4}) + 6\,M_1^3(G) - 11\,M_1^2(G) + 12\,|E| \\
M_1^5(G) &= 5!\,\sigma_G(K_{1,5}) + 10\,M_1^4(G) - 35\,M_1^3(G) + 50\,M_1^2(G) - 48\,|E| \\
M_1^6(G) &= 6!\,\sigma_G(K_{1,6}) + 15\,M_1^5(G) - 85\,M_1^4(G) + 225\,M_1^3(G) \\
&\quad - 274\,M_1^2(G) + 240\,|E| \\
M_1^7(G) &= 7!\,\sigma_G(K_{1,7}) + 21\,M_1^6(G) - 175\,M_1^5(G) + 735\,M_1^4(G) - 1624\,M_1^3(G) \\
&\quad + 1764\,M_1^2(G) - 1440\,|E| \\
M_1^8(G) &= 8!\,\sigma_G(K_{1,8}) + 28\,M_1^7(G) - 322\,M_1^6(G) + 1960\,M_1^5(G) \\
&\quad - 6769\,M_1^4(G) + 13132\,M_1^3(G) - 13068\,M_1^2(G) + 10080\,|E| \\
M_1^9(G) &= 9!\,\sigma_G(K_{1,9}) + 36\,M_1^8(G) - 546\,M_1^7(G) + 4536\,M_1^6(G) - 22449\,M_1^5(G) \\
&\quad + 67284\,M_1^4(G) - 118124\,M_1^3(G) + 109584\,M_1^2(G) - 80640\,|E| \\
M_1^{10}(G) &= 10!\,\sigma_G(K_{1,10}) + 45\,M_1^9(G) - 870\,M_1^8(G) + 9450\,M_1^7(G) \\
&\quad - 63273\,M_1^6(G) + 269325\,M_1^5(G) - 723680\,M_1^4(G) + 1172700\,M_1^3(G) \\
&\quad - 1026576\,M_1^2(G) + 725760\,|E|.
\end{aligned}$$

Theorem 3.2. *Let T be a tree and m an integer such that $2 < m \leq diam(T)$. Then*

$$\sigma_T(P_{m+1}) = \sum_{d(u,v)=m-2} [d_T(u)-1][d_T(v)-1]. \tag{3.4}$$

Proof. We prove (3.4) by induction on the number of vertices of T.

If $|V| = 4$, $|E| = 3$, then T must be either P_4 or $K_{1,3}$ and hence T satisfies (3.4).

For a subtree $T_1 = T - v$, where v is a pendent vertex of T, assume that (3.4) holds for T_1. Therefore the induction hypothesis is

$$\sigma_{T_1}(P_{m+1}) = \sum_{d(x,y)=m-2} [d_{T_1}(x)-1][d_{T_1}(y)-1]. \tag{3.5}$$

Since $uv \notin E(T_1)$ and $uv \in E(T)$, $\sigma_{T_1}(P_{m+1})$ can be expressed as

$$\begin{aligned}
\sigma_{T_1}(P_{m+1}) &= [d_{T_1}(u)-1][d_{T_1}(u_1)-1] + [d_{T_1}(u)-1][d_{T_1}(u_2)-1] \\
&\quad + \cdots + [d_{T_1}(u)-1][d_{T_1}(u_k)-1] + \text{other terms in } T_1
\end{aligned}$$

where $d(u,u_i) = m-2$, $i = 1,2,3,\ldots,k$.

Since for all $x \in V(T_1)\setminus\{u\}$, $d_T(x) = d_{T_1}(x)$ whereas $d_T(u) = d_{T_1}(u)+1$, we have

$$\begin{aligned}
\sigma_{T_1}(P_{m+1}) &= [(d_T(u)-1)-1][d_T(u_1)-1] + [(d_T(u)-1)-1][d_T(u_2)-1] \\
&\quad + \cdots + [(d_T(u)-1)-1][(d_T(u_k)-1)-1] + \text{other terms in } T.
\end{aligned}$$

Therefore, $\sigma_{T_1}(P_{m+1}) = \sigma_T(P_{m+1}) - \sum_{i=1}^{k}[d_T(u_i) - 1]$ and

$$\begin{aligned}\sum_{i=1}^{k}[d_T(u_i) - 1] = & \sum_{\substack{i=1 \\ d(u,u_i)=m-2}}^{k} [(d_{T_1}(u) + 1) - 1][d_{T_1}(u_i) - 1] \\ & - \sum_{\substack{i=1 \\ d(u,u_i)=m-2}}^{k} [d_{T_1}(u) - 1][d_{T_1}(u_i) - 1].\end{aligned}$$

This implies,

$$\begin{aligned}\sigma_T(P_{m+1}) = \sigma_{T_1}(P_{m+1}) + & \sum_{\substack{i=1 \\ d(u,u_i)=m-2}}^{k} [(d_{T_1}(u) + 1) - 1][d_{T_1}(u_i) - 1] \\ & - \sum_{\substack{i=1 \\ d(u,u_i)=m-2}}^{k} [d_{T_1}(u) - 1][d_{T_1}(u_i) - 1]\end{aligned} \tag{3.6}$$

From (3.5) and (3.6) we complete the proof of Theorem 3.2. □

Remark 3.1. The special case of formula (3.4) for $m = 3$, i.e.,

$$\sigma_T(P_4) = \sum_{uv \in E(T)} [d_T(u) - 1][d_T(v) - 1] \tag{3.7}$$

was first established in 2009 [10], and later also in [23, 19, 27]. Its extension to triangle–containing graphs is also known [24]. Within these researches, a relation equivalent to Eq. (3.7), namely

$$M_2(G) = M_1(G) + \sigma_G(P_4) - |E| \tag{3.8}$$

was also reported. For more details on this matter see [15, 16, 13].

Corollary 3.2. *Let T be a tree and m an integer such that $1 < m \leq \mathrm{diam}(T)$. Then* $\sigma_T(P_{m+1}) = \frac{1}{2}\sum_{d(u,v)=m-1}[(d_T(u) - 1) + (d_T(v) - 1)]$.

Corollary 3.3. *Let G be a C_i-free graph $(2 < i \leq m)$. Then*

$$\begin{aligned}\sigma_G(P_{m+1}) &= \sum_{d(u,v)=m-2} [d(u) - 1][d(v) - 1] \\ &= \frac{1}{2} \sum_{d(u,v)=m-1} [(d(u) - 1) + (d(v) - 1)].\end{aligned}$$

Eq. (3.8) can be rewritten as

$$M_2^1(G) = \sigma_G(D_{1,1}) + M_1^2(G) - |E|. \tag{3.9}$$

In the next theorem we show that analogous relations can be found also in the case of higher–order second general Zagreb indices, $M_2^k(G)$, $k \geq 2$.

Theorem 3.3. *Let G be a triangle-free graph. Then*

$$M_2^2(G) = 4\,\sigma_G(D_{2,2}) + 6\,\sigma_G(D_{1,2}) + 9\,M_2^1(G) + M_1^3(G) - 9\,M_1^2(G) + 8\,|E| \tag{3.10}$$

$$M_2^3(G) = 36\,\sigma_G(D_{3,3}) + 144\,\sigma_G(D_{2,2}) + 72\,\sigma_G(D_{2,3}) + 42\,\sigma_G(D_{1,3}) + 84\,\sigma_G(D_{1,2}) + 49\,M_2^1(G) + M_1^4(G) - 49\,M_1^2(G) + 48\,|E|. \tag{3.11}$$

Proof. Using Eq. (1.2), we have

$$\begin{aligned}\sigma_G(D_{1,2}) &= \sum_{uv\in E(G)} \left[\binom{d(u)-1}{1}\binom{d(v)-1}{2} + \binom{d(u)-1}{2}\binom{d(v)-1}{1}\right]\\ &= \frac{1}{2}\sum_{uv\in E(G)} \Big[\big[d(u)^2\,d(v) + d(v)^2\,d(u)\big]\\ &\quad - 6\,d(u)\,d(v) - \big[d(u)^2 + d(v)^2\big] + 5\big[d(u)+d(v)\big] - 4\Big]\\ &= \frac{1}{2}\sum_{uv\in E(G)} \big[d(u)^2\,d(v) + d(v)^2\,d(u)\big]\\ &\quad - \frac{1}{2}\big(6\,M_2^1(G) + M_1^3(G) - 5\,M_1^2(G) + 4\,|E|\big)\end{aligned}$$

i.e.,

$$\sum_{uv\in E(G)} \big[d(u)^2\,d(v) + d(v)^2\,d(u)\big] = 2\,\sigma_G(D_{1,2}) + 6\,M_2^1(G) + M_1^3(G) - 5\,M_1^2(G) + 4\,|E| \tag{3.12}$$

where we used Eq. (2.1) and the definitions (2.3) and (2.4) of the first and second general Zagreb indices.

Using Eq. (1.3) and similar arguments, we obtain

$$\begin{aligned}\sigma_G(D_{2,2}) &= \sum_{uv\in E(G)} \binom{d(u)-1}{2}\binom{d(v)-1}{2}\\ &= \frac{1}{4}\sum_{uv\in E(G)} \Big[d(u)^2\,d(v)^2 + 9\,d(u)\,d(v) + 2\big[d(u)^2 + d(v)^2\big]\\ &\quad - 6\big[d(u)+d(v)\big] + 4 - 3\big[d(u)^2\,d(v) + d(v)^2\,d(u)\big]\Big]\\ &= \frac{1}{4}\Big(M_2^2(G) + 9\,M_2^1(G) + 2\,M_1^3(G) - 6\,M_1^2(G) + 4\,|E|\Big)\\ &\quad - \frac{3}{4}\sum_{uv\in E(G)} \big[d(u)^2\,d(v) + d(v)^2\,d(u)\big]\end{aligned}$$

which combined with Eq. (3.12) yields

$$\sigma_G(D_{2,2}) = \frac{1}{4}\left[M_2^2(G) - 9\,M_2^1(G) - M_1^3(G) + 9\,M_1^2(G) - 8\,|E| - 6\,\sigma_G(D_{1,2})\right]$$

which is equivalent to Eq. (3.10).

The proof of Eq. (3.11) is analogous, yet somewhat more lengthy.

Identities of the same kind as Eqs. (3.10) and (3.11) could be deduced also for second general Zagreb indices $M_2^k(G)$, $k \geq 4$. $\square$

Substituting Eqs. (3.1)–(3.3) and (3.9) back into the relations in Theorem 3.3, we obtain the following.

Corollary 3.4. *Let G be a triangle-free graph. Then*

$$M_2^2(G) = 4\,\sigma_G(D_{2,2}) + 6\,\sigma_G(D_{1,2}) + 6\,\sigma_G(K_{1,3}) + 9\,\sigma_G(P_4) + 6\,\sigma_G(P_3) + |E|$$

$$\begin{aligned} M_2^3(G) = {} & 36\,\sigma_G(D_{3,3}) + 144\,\sigma_G(D_{2,2}) + 72\,\sigma_G(D_{2,3}) + 42\,\sigma_G(D_{1,3}) + 84\,\sigma_G(D_{1,2}) \\ & + 24\,\sigma_G(K_{1,4}) + 36\,\sigma_G(K_{1,3}) + 49\,\sigma_G(P_4) + 14\,\sigma_G(P_3) + |E|. \end{aligned}$$

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