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Abstract

Let $G = (V, E)$ be a simple graph with $n = |V|$ vertices and $m = |E|$ edges; let $d_1, d_2, \ldots, d_n$ denote the degrees of the vertices of G. If $\Delta = \max_i d_i \leq 4$, G is a chemical graph. The first and second Zagreb indices are defined as

$$M_1 = \sum_{i \in V} d_i^2 \quad \text{and} \quad M_2 = \sum_{(i,j) \in E} d_i d_j.$$

We show that for all chemical graphs $M_1/n \leq M_2/m$. This does not hold for all general graphs, connected or not.

Résumé

Soit $G = (V, E)$ un graphe simple avec $n = |V|$ sommets et $m = |E|$ arêtes; soient $d_1, d_2, \ldots, d_n$ les degrés des sommets de G. Si $\Delta = \max_i d_i \leq 4$, G est un graphe chimique. Les premier et second indices de Zagreb sont définis par

$$M_1 = \sum_{i \in V} d_i^2 \quad \text{et} \quad M_2 = \sum_{(i,j) \in E} d_i d_j.$$

Nous montrons que pour tout graphe chimique $M_1/n \leq M_2/m$. Cette relation n'est pas vérifiée pour tous les graphes généraux, connexes ou non.

1 Introduction

We follow the graph theoretical terminology of Berge[1], to which we refer for undefined terms. Let $G = (V, E)$ denote a simple graph with $n = |V|$ vertices and $m = |E|$ edges. Let $d_1, d_2, \ldots, d_n$ denote the degrees of the vertices of G. If $\Delta = \max_i d_i \leq 4$, G is a chemical graph. The first and second Zagreb indices were defined 35 years ago[2] as

$$M_1 = \sum_{i \in V} d_i^2 \quad \text{and} \quad M_2 = \sum_{(i,j) \in E} d_i d_j.$$

They were among the first topological indices[3,4] to be proposed and were often applied, as explained in a recent paper called "The Zagreb Indices 30 Years Later"[5]. That paper and a couple of further surveys[6,7] spurred research on mathematical properties of the Zagreb indices[8–16]. A natural question is to compare the values of the Zagreb indices on the same graph. Observe that, for general graphs, the order of magnitude of M_1 is $O(n^3)$ (n vertices and degrees in $O(n)$, squared) while the order of magnitude of M_1 is $O(n^4)$ ($m = O(n^2)$ edges and degrees in $O(n)$, squared). This suggests to compare M_1/n with M_2/m instead of M_1 and M_2.

Using the system AutoGraphiX[17–19] led to the following:

Conjecture 1 *For all simple connected graphs G,*

$$M_1/n \leq M_2/m \tag{1}$$

and the bound is tight for complete graphs.

As will be shown below, this conjecture turned out to be false for general graphs but true for chemical graphs.

2 Main Result

We now state a result slightly more general than Conjecture 1 and valid for chemical graphs.

Theorem 1 *For all chemical graphs G with order n, size m, first and second Zagreb indices M_1 and M_2,*

$$M_1/n \leq M_2/m.$$

Moreover, the bound is tight if and only if all edges (i, j) have the same pair (d_i, d_j) of degrees or if the graph is composed of disjoint stars S_5 and cycles $C_p, C_q, \ldots$ of any length.

Proof. Let G be a chemical graph, i.e., $\Delta(G) \leq 4$. Denote by m_{ij} the number of edges that connect vertices of degrees i and j and by n_i the number of vertices of degree i in G. On the one hand, we have:

$$\frac{M_1(G)}{n} = \frac{\sum\limits_{v\in V(G)} d(v)^2}{\sum\limits_{i\in N} n_i} = \frac{\sum\limits_{i\in N} n_i \cdot i^2}{\sum\limits_{i\in N} \frac{m_{ij}+\sum_{j\in N} m_{ij}}{i}} = \frac{\sum\limits_{i\in N}\left(\frac{m_{ii}+\sum_{j\in N} m_{ij}}{i}\cdot i^2\right)}{\sum\limits_{i\leq j} m_{ij}\cdot\left(\frac{1}{i}+\frac{1}{j}\right)}$$
$$= \frac{\sum\limits_{i\in N}\left(\left(m_{ii}+\sum\limits_{j\in N} m_{ij}\right)\cdot i\right)}{\sum\limits_{i\leq j} m_{ij}\cdot\left(\frac{1}{i}+\frac{1}{j}\right)} = \frac{\sum\limits_{i\leq j} m_{ij}\cdot(i+j)}{\sum\limits_{i\leq j} m_{ij}\cdot\left(\frac{1}{i}+\frac{1}{j}\right)} \tag{2}$$

On the other hand, we have:

$$\frac{M_2(G)}{m} = \frac{\sum\limits_{(u,v)\in E(G)} d(u)\cdot d(v)}{m} = \frac{\sum\limits_{i\leq j\in N} m_{ij}\cdot i\cdot j}{\sum\limits_{i\leq j\in N} m_{ij}} \tag{3}$$

Putting (2) and (3) in (1), we get:

$$\frac{\sum\limits_{i\leq j} m_{ij}\cdot(i+j)}{\sum\limits_{i\leq j} m_{ij}\cdot\left(\frac{1}{i}+\frac{1}{j}\right)} \leq \frac{\sum\limits_{i\leq j\in N} m_{ij}\cdot i\cdot j}{\sum\limits_{i\leq j\in N} m_{ij}},$$

or equivalently:

$$\frac{\sum\limits_{i\leq j} m_{ij}\cdot(i+j)}{\sum\limits_{k\leq l} m_{kl}\cdot\left(\frac{1}{k}+\frac{1}{l}\right)} \leq \frac{\sum\limits_{i\leq j\in N} m_{ij}\cdot i\cdot j}{\sum\limits_{k\leq l\in N} m_{kl}}.$$

Hence

$$\left[\sum_{i\leq j\in N} m_{ij}\cdot i\cdot j\right]\cdot\left[\sum_{k\leq l} m_{kl}\cdot\left(\frac{1}{k}+\frac{1}{l}\right)\right] - \left[\sum_{i\leq j} m_{ij}\cdot(i+j)\right]\cdot\left[\sum_{k\leq l\in N} m_{kl}\right] \geq 0$$

and

$$\sum_{\substack{i\leq j\\ k\leq l\\ i,j,k,l\in N}} \left[\left(i\cdot j\cdot\left(\frac{1}{k}+\frac{1}{l}\right) - i - j\right)\cdot m_{ij}\cdot m_{kl}\right] \geq 0.$$

Now, collecting in the same summand cases where roles of (i, j) and (k, l) are reversed one gets:

$$\sum_{\substack{i \le j \\ k \le l \\ ](i,j),(k,l) \subseteq N^2}} \left[\left(i \cdot j \cdot \left(\frac{1}{k} + \frac{1}{l} \right) + k \cdot l \cdot \left(\frac{1}{i} + \frac{1}{j} \right) - i - j - k - l \right) \cdot m_{ij} \cdot m_{kl} \right] \ge 0$$

and

$$\sum_{\substack{i \le j \\ k \le l \\ (i,j),(k,l) \subseteq N^2}} \left[\left(i^2 j^2 l + i^2 j^2 k + k^2 l^2 j + k^2 l^2 i - i^2 jkl - ij^2 kl - ijk^2 l - ijkl^2 \right) \cdot \frac{m_{ij} \cdot m_{kl}}{i \cdot j \cdot k \cdot l} \right] \ge 0. \quad (4)$$

It remains to prove relation (4). It is sufficient to show that:

$$g(i, j, k, l) = i^2 j^2 l + i^2 j^2 k + k^2 l^2 j + k^2 l^2 i - i^2 jkl - ij^2 kl - ijk^2 l - ijkl^2 \ge 0$$

for each $(i, j), (k, l) \subseteq \{1, 2, 3, 4\}^2$. The values of $g(i, j, k, l)$ are presented in Table 1.

One can see that all entries are non-negative, which proves the claim.

To show when relation (3) is satisfied as an equality, consider again function $g(i, j, k, l)$ and its values as given in Table 1. To have equality in (1), one must have $g(i, j, k, l) = 0$ for all $m_{ij} \cdot m_{kl} > 0$. This can only happen if there is a single pair of degrees for all edges, or if either $i = k = 1$, $j = l = 4$ or $i = j = k = l = 2$ for all edges. This last case corresponds to a set of disjoint stars S_5 and cycles $C_p, C_q, \ldots$ of any length. □

Table 1: Value of the function $g(i, j, k, l)$

		$\{i,j\}$									
		$\{1,1\}$	$\{1,2\}$	$\{1,3\}$	$\{1,4\}$	$\{2,2\}$	$\{2,3\}$	$\{2,4\}$	$\{3,3\}$	$\{3,4\}$	$\{4,4\}$
$\{k,l\}$	$\{1,1\}$	0	1	4	9	12	35	70	96	187	360
	$\{1,2\}$	1	0	1	4	8	32	72	105	220	448
	$\{1,3\}$	4	1	0	1	4	27	70	108	243	520
	$\{1,4\}$	9	4	1	0	0	20	64	105	256	576
	$\{2,2\}$	12	8	4	0	0	8	32	60	160	384
	$\{2,3\}$	35	32	27	20	8	0	8	27	108	320
	$\{2,4\}$	70	72	70	64	32	8	0	6	64	256
	$\{3,3\}$	96	105	108	105	60	27	6	0	27	168
	$\{3,4\}$	187	220	243	256	160	108	64	27	0	64
	$\{4,4\}$	360	448	520	576	384	320	256	168	64	0

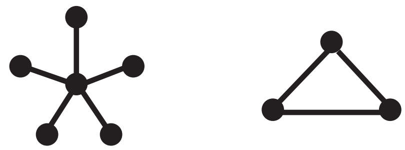

Figure 1: A non-connected counter-example to Conjecture 1

To finish, we show that (1) does not hold for general graphs. If G is not connected the condition $\Delta \leq 4$ cannot be relaxed. Indeed, let us observe the graph G_1 presented in Figure 1.

We have:

$$\frac{M_1(G_1)}{n} = \frac{5 \cdot 1^2 + 1 \cdot 5^2 + 3 \cdot 2^2}{9} = \frac{42}{9} = \frac{14}{3} = 4.66\ldots$$
$$\frac{M_2(G_1)}{m} = \frac{5 \cdot (5 \cdot 1) + 3 \cdot (2 \cdot 2)}{8} = \frac{37}{8} = 4.625.$$

Obviously, relation (1) does not hold.

Finding a connected counter-example is a bit more difficult.

Let G'_1 be the disjoint union of $K(U_1, V_1), \ldots, K(U_4, V_4)$ where each $K(X, Y)$ is a complete bipartite graph with classes X and Y. Let $|U_1| = |U_2| = 3$, $|V_1| = |V_2| = 10$ and $|U_3| = |U_4| = |V_3| = |V_4| = 5$.

Obviously, we have $n_3(G'_1) = 20$, $n_{10}(G'_1) = 6$ and $n_5(G'_1) = 20$. Also, $m_{3,10}(G'_1) = 60$ and $m_{5,5} = 50$.

Let $u_i, u'_i \in U_i$ and $v_i, v'_i \in V_i$ be arbitrary (pairwise different) but fixed vertices. Let G'_2 be the graph defined by:

$$G'_2 = G'_1 - \{u_1v_1, u'_2v'_2, u_2v_2, u'_3v'_3, u_3v_3, u_4v_4\} \cup \{u_1v'_2, u'_2v_1, u_2v'_3, u'_3v_2, u'_3v_4, u_4v'_3\}$$

which is illustrated by Figure 2 (dashed lines are deleted and solid lines are added).

Obviously, no vertex has changed its degree. Note that $m_{3,10}(G'_2) = m_{3,10}(G'_1) - 3 + 2 = 59$; $m_{5,5}(G'_2) = m_{5,5}(G'_2) - 3 + 2 = 49$, $m_{5,10}(G'_2) = 1$ and $m_{3,5}(G'_2) = 1$.

We have:

$$\frac{M_1(G'_2)}{n} = \frac{20 \cdot 5^2 + 6 \cdot 10^2 + 20 \cdot 3^2}{20 + 6 + 20} = \frac{1280}{46} \approx 27.826$$
$$\frac{M_2(G'_2)}{m} = \frac{59 \cdot (3 \cdot 10) + 49 \cdot (5 \cdot 5) + 1 \cdot (3 \cdot 5) + 1 \cdot (5 \cdot 10}{59 + 49 + 1 + 1} = \frac{1770 + 1225 + 15 + 50}{110}$$
$$= \frac{3060}{110} \approx 27.818.$$

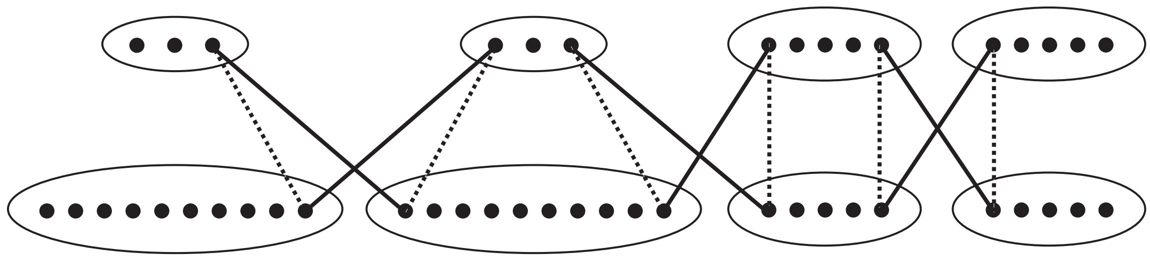

Figure 2: A connected counter-example to Conjecture 1

3 Conclusion

The Zagreb indices M_1 and M_2, divided by the order n and the size m respectively, have been compared. The AutoGraphiX system conjectured that $M_1/n \leq M_2/m$ for simple connected graphs. A counter-example with 48 vertices (and beyond the range of AutoGraphiX) shows that this is not so. However, we proved that this relation holds for chemical graphs, which are the most interesting in practice.

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