CROATICA CHEMICA ACTA
CCACAA **80** (2) 165–168 (2007)

ISSN-0011-1643
CCA-3156
Original Scientific Paper

Comparing the Zagreb Indices*

Pierre Hansen[a] and Damir Vukičević[b,]**

[a]*GERAD and Department of Management Sciences, HEC Montréal 3000, Chemin de la Côte-Sainte-Catherine, Montréal (Québec) Canada, H3T 2A7*

[b]*Department of Mathematics, University of Split, Nikole Tesle 12, HR-21000 Split, Croatia*

RECEIVED SEPTEMBER 21, 2006; REVISED FEBRUARY 12, 2007; ACCEPTED FEBRUARY 14, 2007

Keywords
extremal graphs
Zagreb index
AGX
chemical graphs

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.

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 called a chemical graph. The first and second Zagreb indices were defined 35 years ago[2] as:

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

They were among the first topological indices[3–6] to be proposed and were often applied, as explained in a recent paper called »The Zagreb Indices 30 Years Later«.[7] That paper and a couple of further surveys[8,9] spurred research on mathematical properties of the Zagreb indices.[10–18] A natural issue 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 comparing M_1/n with M_2/m instead of M_1 and M_2.

Use of the AutoGraphiX system[19–21] 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.

* Dedicated to Professor Haruo Hosoya in happy celebration of his 70[th] birthday.
** Author to whom correspondence should be addressed. (E-mail: vukicevi@pmfst.hr)

MAIN RESULT

We now state a result slightly more general than the Conjecture 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:

$M_1/n \le M_2/m$.

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, … of any length.

Proof: Let G be a chemical graph, *i.e.*, $\Delta(G) \le 4$. 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:

$$\frac{M_1(G)}{n} = \frac{\sum\limits_{v\in V(G)} d(v)^2}{\sum\limits_{i\in N} n_i} = \frac{\sum\limits_{i\in N} n_i \cdot i^2}{\sum\limits_{i\in N} \frac{m_i + \sum\limits_{j\in N} m_{ij}}{i}} =$$

$$\frac{\sum\limits_{i\in N}\left(\frac{m_i + \sum\limits_{j\in N} m_{ij}}{i}\cdot i^2\right)}{\sum\limits_{i\le j} m_{ij}\cdot\left(\frac{1}{i}+\frac{1}{j}\right)} = \frac{\sum\limits_{i\in N}\left(\left(m_{ii} + \sum\limits_{j\in N} m_{ij}\right)\cdot i\right)}{\sum\limits_{i\le j} m_{ij}\cdot\left(\frac{1}{i}+\frac{1}{j}\right)} =$$

$$\frac{\sum\limits_{i\le j} m_{ij}\cdot(i+j)}{\sum\limits_{i\le j} m_{ij}\cdot\left(\frac{1}{i}+\frac{1}{j}\right)} \tag{2}$$

On the other hand, we have:

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

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

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

or equivalently:

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

Hence:

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

$$\left[\sum_{i\le j} m_{ij}\cdot(i+j)\right]\left[\sum_{k\le l\in N} m_{kl}\right] \ge 0$$

and

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

Now, collecting in the same summand the cases where roles of (i, j) and (k, l) are reversed, one gets relation (4).

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

and

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

TABLE I. Value of 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

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

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

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

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

To show when relation (4) is satisfied as an equality, consider again function $g(i,j,k,l)$ and its values as given in Table I. 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, … of any length.

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 graph G_1 presented in Figure 1.

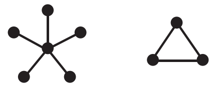

Figure 1. A non-connected counterexample to Conjecture 1.

We have:

$$\frac{M_1(G_1)}{n} = \frac{5 \cdot 1^2 + 1 \cdot 5^2 + 3 \cdot 2^2}{9} = \frac{42}{9} = \frac{14}{3} = 4.66\ ...$$

$$\frac{M_2(G_1)}{m} = \frac{5 \cdot (5 \cdot 1) + 3 \cdot (2 \cdot 2)}{8} = \frac{37}{8} = 4.625.$$

Obviously, the relation (1) does not hold.

Finding a connected counterexample is a bit more difficult.

Let G'_1 be the disjoint union of $K(U_1,V_1)$, …, $K(U_4,V_4)$ 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 $m_{5,5}(G'_1) = 50$.

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 in Figure 2 (dashed lines are deleted and solid lines are added).

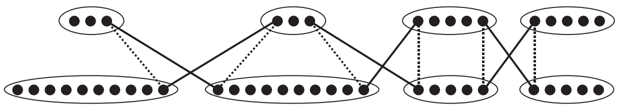

Figure 2. A connected counterexample to Conjecture 1.

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:

$$\frac{M_1(\mathrm{G'}_2)}{n} = \frac{20\cdot 5^2 + 6\cdot 10^2 + 20\cdot 3^2}{20+6+20} = \frac{1280}{46} \approx 27.826$$

$$\frac{M_2(\mathrm{G'}_2)}{m} = \frac{59\cdot(3\cdot 10)+49\cdot(5\cdot 5)+1\cdot(3\cdot 5)+1\cdot(5\cdot 10)}{59+49+1+1} =$$

$$\frac{1770+1225+15+50}{110} = \frac{3060}{110} \approx 27.818.$$

CONCLUSION

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

REFERENCES

1. C. Berge, *Graphs and Hypergraphs*, Macmillan, London, 1973.
2. I. Gutman and N. Trinajstić, *Chem. Phys. Lett.* **17** (1972) 535–538.
3. A. T. Balaban, I. Motoc, D. Bonchev, and O. Mekenyan, *Topics Curr. Chem.* **114** (1983) 21–55.
4. R. Todeschini and V. Consonni, *Handbook of Molecular Descriptors*, Wiley-VCH, Weinheim, 2000.
5. J. Devillers and A. T. Balaban (Eds.), *Topological Indices and Related Descriptors in QSAR and QSPR*, The Netherlands, Gordon and Breach, 1999.
6. M. Karelson, *Molecular Descriptors in QSAR/QAPR*, Wiley-Interscience, New York, 2000.
7. S. Nikolić, G. Kovačević, A. Milićević, and N. Trinajstić, *Croat. Chem. Acta* **76** (2003) 113–124.
8. I. Gutman and K. C. Das, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 83–92.
9. B. Zhou and I. Gutman, *MATCH Commun. Math. Comput. Chem.* **54** (2005) 233–239.
10. K. C. Das, *Kragujevac J. Math.* **25** (2003) 31–49.
11. K. C. Das and I. Gutman, *MATCH Commun. Math. Comput. Chem.* **52** (2004) 103–112.
12. D. de Caen, *Discr. Math.* **185** (1998) 245–248.
13. J. S. Li and Y. L. Pang, *Lin. Algebra Appl.* **328** (2001) 253–263.
14. B. Liu and I. Gutman, *MATCH Commun. Math. Comput. Chem.* **55** (2006) 439–446.
15. P. Hansen, H. Mélot, and I. Gutman, *MATCH Commun. Math. Comput. Chem.* **53** (2005) 221–232.
16. S. Zhang and H. Zhang, *MATCH Commun. Math. Comput. Chem.* **55** (2006) 427–438.
17. B. Zhou. *MATCH Commun. Math. Comput. Chem.* **52** (2004) 113–118.
18. B. Zhou and D. Stevanović, *MATCH Commun. Math. Comput. Chem.* **56** (2006) 571–577.
19. M. Aouchiche, J. M. Bonnefoy, A. Fidahoussen, G. Caporossi, P. Hansen, L. Hiesse, J. Lacheré, and A. Monhait, *Variable Neighborhood Search for Extremal Graphs.* 14. *The AutoGraphiX 2 system,* in: L. Liberti and N. Maculan (Eds.), *Global Optimization: From Theory to Implementation*, Springer, 2005.
20. G. Caporossi and P. Hansen, *Discr. Math.* **212** (2000) 29–44.
21. G. Caporossi and P. Hansen, *Discr. Math.* **276** (2004) 81–94.

SAŽETAK

Usporedba zagrebačkih indeksa

Pierre Hansen i Damir Vukičević

Neka je G = (V, E) jednostavan graf s $n = |V|$ vrhova i $m = |E|$ bridova; neka $d_1, d_2, \ldots, d_n$ označavaju stupnjeve vrhova u G. Ako je $\Delta = \max_i d_i \le 4$, tada G nazivamo kemijskim grafom. Prvi i drugi zagrebački indeks definirani su formulama:

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

U radu je dokazano da je $M_1/n \le M_2/m$ za sve kemijske grafove, te da se ova tvrdnja ne može poopćiti na sve grafove, kako povezane tako i nepovezane.