MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **97** (2027) 1139–1146
ISSN: 0340–6253
doi: 10.46793/match.97-3.05226

New Inequalities Linking the First and Second Zagreb Indices

El-Mehdi Mehiri[a,*]

[a] *Mines Saint-Etienne, CMP, Department of Manufacturing Sciences and Logistics, F-13120 Gardanne, France*

elmehdi.mehiri@emse.fr, mehiri314@gmail.com

(Received February 9, 2026)

Abstract

The first and second Zagreb indices are among the most studied vertex–degree–based graph invariants and play an important role in both chemical graph theory and extremal graph analysis. In this paper we establish new inequalities that directly relate these two indices under general structural assumptions.

1 Introduction

Vertex–degree–based topological indices constitute one of the central themes of chemical graph theory and extremal graph invariants. Among the oldest and most intensively investigated of these descriptors are the first and second Zagreb indices, introduced in the early 1970s by Gutman and Trinajstić in connection with studies of molecular φ–electron energy [5]. For a simple graph $G = (V, E)$ with vertex degrees $\{d(v)\}_{v \in V}$, these indices are defined by

$$M_1(G) = \sum_{v \in V} d(v)^2, \qquad M_2(G) = \sum_{uv \in E} d(u)d(v).$$

*Corresponding author.

A major direction of research concerns extremal properties and bounds for the Zagreb indices in terms of structural parameters such as the number of vertices and edges, extremal degrees, clique number, or spectral quantities. Numerous inequalities and characterizations of extremal graphs have been established; see for example the survey of Borovićanin et *al.* [3] and references therein. Typical results provide lower and upper bounds on M_1 or M_2 in terms of n, m, Δ, δ, or describe graphs attaining extremal values. For instance, bounds depending on degree parameters and edge counts were derived in [10], while structural constraints such as forbidden cliques or prescribed clique number were investigated in [12, 13]. The study of extremal behavior has thus become a standard tool for understanding how graph structure influences these indices.

Another line of research examines relationships between the two Zagreb indices. Comparisons between normalized quantities M_1/n and M_2/m, including conjectured Zagreb indices inequality $M_1/n \leq M_2/m$, and counterexamples, were investigated in [4,6,7]. Such results highlight the subtle interplay between the purely degree–sequence nature of M_1 and the adjacency–dependent structure encoded by M_2.

Motivated by this body of work, the aim of the present paper is to establish new inequalities directly relating the first and second Zagreb indices.

Throughout this paper, $G = (V, E)$ denotes a finite simple graph with $n = |V|$ vertices and $m = |E|$ edges. The degree of a vertex v is denoted by $d(v)$, and we write

$$\Delta = \max_{v \in V} d(v), \qquad \delta = \min_{v \in V} d(v).$$

We recall the following expression of the fist Zagreb index,

$$M_1(G) = \sum_{uv \in E(G)} \big(d(u) + d(v)\big). \tag{1}$$

Which comes from the fact that each vertex v contributes $d(v)$ to the sum $d(u) + d(v)$ for each of the $d(v)$ edges incident to v, yielding a total contribution of $d(v)^2$.

2 Spectral-radius based inequality

Denote by $A = A(G)$ the adjacency matrix of G. Let the degree vector

$$\mathbf{d} = (d_1, \ldots, d_n)^\top,$$

and spectral radius $\rho(G) = \max\{|\lambda_1|, \ldots, |\lambda_n|\}$, where λ_i is i-th eigenvalue of A. Recall that

$$M_1(G) = \|\mathbf{d}\|_2^2, \tag{2}$$

and that M_2 satisfies the following quadratic form identity.

Lemma 1. *For every graph G,*

$$\mathbf{d}^\top A\,\mathbf{d} \;=\; 2\,M_2(G). \tag{3}$$

Proof. We have

$$\begin{aligned}\mathbf{d}^\top A\,\mathbf{d} &= \sum_{i=1}^{n}\sum_{j=1}^{n} d_i\,A_{ij}\,d_j = \sum_{ij\in E(G)} d_i d_j + \sum_{ji\in E(G)} d_j d_i \\ &= 2\sum_{ij\in E(G)} d_i d_j = 2M_2(G)\;. \qquad \blacksquare\end{aligned}$$

Theorem 1. *For every graph G,*

$$M_2(G) \;\le\; \frac{\rho(G)}{2}\,M_1(G). \tag{4}$$

If G is connected, then equality holds if and only if $\mathbf{d}$ is a Perron eigenvector, i.e. $A\mathbf{d} = \rho(G)\mathbf{d}$. In particular, every connected regular graph satisfies equality, but there are also connected irregular graphs with equality.

Proof. By Lemma 1 and the Rayleigh quotient inequality [11, Chapter 4],

$$2M_2(G) = \mathbf{d}^\top A\,\mathbf{d} \;\le\; \rho(G)\,\mathbf{d}^\top\mathbf{d} = \rho(G)\,\|\mathbf{d}\|_2^2 = \rho(G)\,M_1(G),$$

which proves the stated bound.

Assume now that G is connected. If equality holds, then $\mathbf{d}$ attains the maximum Rayleigh quotient, hence $\mathbf{d}$ is an eigenvector of A for $\rho(G)$. Since A is irreducible and nonnegative, the Perron–Frobenius eigenvector for $\rho(G)$ is unique up to scaling and has all positive entries; thus $\mathbf{d}$ must be proportional to this Perron vector. In particular, for every vertex i,

$$(A\mathbf{d})_i = \sum_{j \sim i} d_j = \rho(G)\, d_i.$$

If all degrees are equal, the graph is regular and the above holds. Conversely, if the above holds with $\mathbf{d}$ being the degree vector, then summing over all vertices and using connectivity forces degree uniformity (equivalently, $\mathbf{d}$ must be proportional to $\mathbf{1}$, the Perron vector of a regular connected graph), hence G is regular. ■

Corollary. *For every graph G with maximum degree Δ,*

$$M_2(G) \;\leq\; \frac{\Delta}{2}\, M_1(G). \tag{5}$$

If G is connected, equality holds if and only if G is Δ-regular.

Proof. It is standard that $\rho(G) \leq \Delta$ for any simple graph. Combine with Theorem 1. ■

The result of Corollary 2 is already known and was stated as a proposition by Ilić and Stevanović in [8, Proposition 2.4].

3 Universal inequality

Theorem 2. *For every simple graph G,*

$$M_2(G) \;\leq\; \frac{M_1(G)^2}{4}. \tag{6}$$

Equality holds if and only if $d(u) = d(v)$ for every edge $uv \in E(G)$ and the quantities $\sqrt{d(u)d(v)}$ are constant over all edges (in particular, this includes regular graphs or disjoint unions of regular components of the same degree).

Proof. Set $a_{uv} = \sqrt{d(u)d(v)}$ for each edge $uv \in E(G)$. Then

$$M_2(G) = \sum_{uv \in E(G)} a_{uv}^2.$$

Since for any nonnegative numbers a_i we have

$$\sum_i a_i^2 \leq \Big(\sum_i a_i\Big)^2,$$

it follows that

$$M_2(G) \leq \left(\sum_{uv \in E(G)} \sqrt{d(u)d(v)}\right)^2.$$

By the arithmetic–geometric mean inequality,

$$\sqrt{d(u)d(v)} \leq \frac{d(u)+d(v)}{2}.$$

Summing over all edges and applying (1),

$$\sum_{uv \in E(G)} \sqrt{d(u)d(v)} \leq \frac{1}{2} \sum_{uv \in E(G)} (d(u)+d(v)) = \frac{M_1(G)}{2}.$$

Combining the inequalities yields

$$M_2(G) \leq \frac{M_1(G)^2}{4}.$$

Equality holds precisely when equality is achieved in both steps: (i) all a_{uv} are proportional (so their squares sum maximally), and (ii) $d(u) = d(v)$ for every edge uv. This forces constant degree products across edges, giving the stated characterization. ■

4 Extremal-degrees based inequalities

In this section we derive two inequalities that relate the second Zagreb index $M_2(G)$ to the first Zagreb index $M_1(G)$ and to extremal degree parameters.

Theorem 3. *Let G be a graph with minimum degree δ. Then*

$$M_2(G) \;\geq\; \delta\, M_1(G) - m\delta^2. \tag{7}$$

Equality holds if and only if each edge of G has at least one endpoint of degree δ.

Proof. For any edge $uv \in E(G)$ we have

$$(d(u) - \delta)(d(v) - \delta) \geq 0,$$

since $d(u), d(v) \geq \delta$. Expanding,

$$d(u)d(v) \geq \delta(d(u) + d(v)) - \delta^2.$$

Summing over all edges gives

$$M_2(G) \geq \delta \sum_{uv \in E(G)} (d(u) + d(v)) - m\delta^2.$$

Using (1),

$$M_2(G) \geq \delta M_1(G) - m\delta^2.$$

Equality holds if and only if $(d(u)-\delta)(d(v)-\delta) = 0$ for every edge, meaning that each edge has an endpoint of degree δ. ■

Theorem 4. *Let G be a graph with maximum degree Δ. Then*

$$M_2(G) \;\leq\; \Delta\, M_1(G) - m\Delta^2. \tag{8}$$

Equality holds if and only if each edge of G has at least one endpoint of degree Δ.

Proof. For any edge $uv \in E(G)$,

$$(\Delta - d(u))(\Delta - d(v)) \geq 0,$$

since $d(u), d(v) \leq \Delta$. Expanding,

$$d(u)d(v) \leq \Delta(d(u) + d(v)) - \Delta^2.$$

Summing over all edges,

$$M_2(G) \leq \Delta \sum_{uv \in E(G)} (d(u) + d(v)) - m\Delta^2.$$

Applying (1) yields

$$M_2(G) \leq \Delta M_1(G) - m\Delta^2.$$

Equality holds when $(\Delta - d(u))(\Delta - d(v)) = 0$ for each edge, i.e., every edge has an endpoint of maximum degree. ■

References

[1] H. Abdo, D. Dimitrov, T. Réti, D. Stevanović, Estimating the spectral radius of a graph by the second Zagreb index, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 741–751.

[2] H. Abeledo, G. Atkinson, Polyhedral combinatorics of benzenoid problems, in: R. E. Bixby, E. A. Boyd, R. Z. Ríos–Mercado (Eds.), *Integer Programming and Combinatorial Optimization*, Springer, Berlin, 1998, pp. 202–212.

[3] B. Borovićanin, K. C. Das, B. Furtula, I. Gutman, Bounds for Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **78** (2017) 17–100.

[4] A. Ghalavand, On a conjecture about comparing the first and second Zagreb indices of graphs, *MATCH Commun. Math. Comput. Chem.* **96** (2026) 441–452.

[5] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535–538.

[6] P. Hansen, D. Vukičević, Comparing the Zagreb indices, *Croat. Chem. Acta* **80** (2007) 165–168.

[7] B. Horoldagva, S. G. Lee, Comparing Zagreb indices for connected graphs, *Discr. Appl. Math.* **158** (2010) 1073–1078.

[8] A. Ilić, D. Stevanović, On comparing Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **62** (2009) 681–687.

[9] X. Li, Y. Shi, I. Gutman, *Graph Energy*, Springer, New York, 2012.

[10] E. I. Milovanović, I. Milovanović, Sharp bounds for the first Zagreb index and first Zagreb coindex, *Miskolc Math. Notes* **16** (2015) 1017–1024.

[11] R. A. Horn, C. R. Johnson, *Matrix Analysis*, Cambridge Univ. Press, Cambridge, 2012.

[12] K. Xu, The Zagreb indices of graphs with a given clique number, *Appl. Math. Lett.* **24** (2011) 1026–1030.

[13] B. Zhou, Remarks on Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 591–596.