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Variable Zagreb Indices and Karamata's Inequality

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Abstract

For a simple graph G with n vertices and m edges, the inequality $M_1(G)/n \leq M_2(G)/m$, where $M_1(G)$ and $M_2(G)$ are the first and the second Zagreb indices of G, is known as Zagreb indices inequality. Generalization of these indices gives first ${}^\lambda M_1(G)$ and second ${}^\lambda M_2(G)$ variable Zagreb indices. Vukičević in [13] has given an incomplete proof for the claim: for all simple graphs and all $\lambda \in [0, \frac{1}{2}]$, holds ${}^\lambda M_1(G)/n \leq^\lambda M_2(G)/m$. Here we present a complete proof using Karamata's inequality.

1 Introduction

The concept of the variable molecular descriptors was proposed as an alternative way of characterizing heteroatoms in molecules, but also to assess the structural differences, such as, for example, the relative role of carbon atoms of acyclic and cyclic parts in alkylcycloalkanes. The idea behind the variable molecular descriptors is that the variables are determined during the regression so that the standard error of estimate for a studied property is as small

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as possible. Several molecular descriptors, have already been generalized in their variable forms, but here we will only pay attention to Zagreb indices. These indices have been used to study molecular complexity, chirality, ZE-isomerism and hetero-systems. Overall, Zagreb indices exhibit a potential applicability for deriving multi-linear regression models.

Let $G = (V, E)$ be a simple graph with $n = |V|$ vertices and $m = |E|$ edges. For $v \in V$, $d(v)$ is its degree. The first Zagreb index $M_1(G)$ and the second Zagreb $M_2(G)$ index are among the oldest topological indices [1, 3, 5] defined in 1972 by Gutman and Trinajstić [4] as follows:

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

Similarly, first and second variable Zagreb indices are defined by

$$^{\lambda}M_1(G) = \sum_{v \in V} d(v)^{2\lambda} \quad \text{and} \quad ^{\lambda}M_2(G) = \sum_{uv \in E} d^{\lambda}(u)d^{\lambda}(v),$$

where λ is a real number. For the sake of simplicity, we use $^{\lambda}M_1$ and $^{\lambda}M_2$ instead of $^{\lambda}M_1(G)$ and $^{\lambda}M_2(G)$, respectively.

The Zagreb indices are generally related to the inequality $M_1(G)/n \leq M_2(G)/m$ and the question: When does this inequality hold? Similarly to this, many mathematicians analyzed the inequality

$$\frac{^{\lambda}M_1(G)}{n} \leq \frac{^{\lambda}M_2(G)}{m} \tag{1}$$

when $\lambda \in [0, 1]$, and showed that it is true for the following cases: all chemical graphs [13], all trees [12], all unicyclic graphs [6]. For more results on this topic see [7, 9, 10, 14]. Vukičević [13] also analyzed the inequality (1) and showed that it does not holds for $\lambda \in [\frac{\sqrt{2}}{2}, 1]$. The case when $\lambda \in [\frac{1}{2}, \frac{\sqrt{2}}{2}]$ is still an open problem. In the same paper an incomplete proof of the following theorem is given:

Theorem 1.1. *For all graphs G and all $\lambda \in [0, \frac{1}{2}]$, holds $^{\lambda}M_1/n \leq ^{\lambda} M_2/m$.*

Since we discuss sufficient conditions for (1) to hold, for the sake of simplicity we denote by $m_{i,j}$ the number of edges that connect vertices of degrees i and j in the graph G. Then, as shown in [13]:

$$^{\lambda}M_1/n -^{\lambda} M_2/m = \sum_{\substack{i \leq j \\ i,j \in \mathbb{N}}} f(i,j)m_{ij}^2 + \sum_{\substack{i \leq j, k \leq l \\ (i,j) \neq (k,l)}} g(i,j,k,l)m_{ij}m_{kl}, \tag{2}$$

where the functions f and g are defined in the following way:

$$f(i,j) = i^\lambda j^\lambda \left(\frac{1}{i} + \frac{1}{j}\right) - i^{2\lambda-1} - j^{2\lambda-1}, \tag{3}$$

and

$$g(i,j,k,l) = i^\lambda j^\lambda \left(\frac{1}{k} + \frac{1}{l}\right) + k^\lambda l^\lambda \left(\frac{1}{i} + \frac{1}{j}\right) - i^{2\lambda-1} - j^{2\lambda-1} - k^{2\lambda-1} - l^{2\lambda-1}. \tag{4}$$

In order to examine whether the inequality (1) holds, one can consider whether ${}^\lambda M_2/m - {}^\lambda M_1/n$ is non-negative. If $f(i,j) < 0$ or $g(i,j,k,l) < 0$ for some integers i,j,k,l, then there is a graph G such that the inequality (1) does not hold. The construction of such graph can be done in the same way as the one for Zagreb indices in [13].

The proof of the Theorem 1.1 is based on the following two lemmas:

Lemma 1.1. *Let i and j be different natural numbers and let $f(i,j)$ is defined by (3). Then, $f(i,j) \geq 0$ for $\lambda \in [0,1]$ and $f(i,j) < 0$ for $\lambda \in \mathbb{R}\backslash[0,1]$.*

Lemma 1.2. *Let i,j,k and j be different natural numbers and let $\lambda \in [0, \frac{1}{2}]$. Then the function $g(i,j,k,l)$ defined by (4) in non-negative.*

Without loss of generality, we may assume that $i = \max\{j,k,l\}$ and that $k \geq l$. Now, there are three possible orderings:

(a) $i \geq j \geq k \geq l$, (b) $i \geq k \geq j \geq l$, (c) $i \geq k \geq l \geq j$.

The cases (a) and (b) are proven in [13], even more for these orderings holds $g(i,j,k,l) \geq 0$ for all $\lambda \in [0,1]$.

The incompleteness in the proof of Lemma 1.2 is for the third ordering. Namely, $\dfrac{\partial g(i,j,k,l)}{\partial i}$ is not non-negative [13] in the case (c).

2 Proof of Theorem 1.1

By the above discussion, one can easily see that the main problem here is determining the sign of g for $\lambda \in [0, \frac{1}{2}]$. In order to do that, we will use some already known results [8].

Lemma 2.1. [Karamata's inequality] Let $U \subseteq \mathbb{R}$ be an open interval and $f : U \to U$ be a convex function. Let $a_1 \geq a_2 \geq \ldots \geq a_n$ and $b_1 \geq b_2 \geq \ldots \geq b_n$ belong to U are such that $a_1 + a_2 + \ldots + a_i \geq b_1 + b_2 + \ldots + b_i$ for every $i \in \{1,2,\ldots,n\}$ with equality for $i = n$. Then $f(a_1) + f(a_2) + \ldots + f(a_n) \geq f(b_1) + f(b_2) + \ldots + f(b_n)$.

Since monotonicity of the $a's$ only strengthens the majorizing conditions $a_1 + a_2 + \ldots + a_i \geq b_1 + b_2 + \ldots + b_i$ for every $i \in \{1, 2, \ldots, n\}$ with equality for $i = n$, we have that the same inequality holds without any restrictions on order on the a's.

If in addition $U = \mathbb{R}$ and the function f is non-decreasing on U, then the majorizing conditions can be further relaxed from "with equality for $i = n$". Namely if $a_1 + a_2 + \ldots + a_n > b_1 + b_2 + \ldots + b_n$, then we take $a'_n = b_1 + b_2 + \ldots + b_n - a_1 - a_2 - \ldots - a_{n-1}$. With a'_n instead of a_n we have that all the needed for Karamata's is satisfied and $f(a_n) \geq f(a'_n)$, which goes on our hand.

These comments explain how the following is derived from Lemma 2.1.

Lemma 2.2. [Majorizing inequality] Let $f : \mathbb{R} \to \mathbb{R}$ be a non-decreasing convex function. Let $a_1, a_2, \ldots, a_n$ and $b_1 \geq b_2 \geq \ldots \geq b_n$ be reals such that $a_1+a_2+\ldots+a_i \geq b_1+b_2+\ldots+b_i$ for every $i \in \{1, 2, \ldots, n\}$. Then $f(a_1) + f(a_2) + \ldots + f(a_n) \geq f(b_1) + f(b_2) + \ldots + f(b_n)$.

A Lemma 2.2 will be are use to prove the following result.

Theorem 2.1. *Let $a, b, c, d \in \mathbb{R}^+$ and $x \in [0, \frac{1}{2}]$. Then*

$$a^x b^x (\frac{1}{c} + \frac{1}{d}) + c^x d^x (\frac{1}{a} + \frac{1}{b}) \geq a^{2x-1} + b^{2x-1} + c^{2x-1} + d^{2x-1}.$$

Proof. Put $A = -\log_t a$, $B = -\log_t b$, $C = -\log_t c$, $D = -\log_t d$, for a fixed real $t > 1$. Then this inequality takes on the form

$$t^{A-(C+D)x} + t^{B-(C+D)x} + t^{C-(A+B)x} + t^{D-(A+B)x} \geq t^{(1-2x)A} + t^{(1-2x)B} + t^{(1-2x)C} + t^{(1-2x)D}.$$

Put $a_1 = A - (C + D)x$, $a_2 = B - (C + D)x$, $a_3 = C - (A + B)x$, $a_4 = D - (A + B)x$ and $b_1 = (1 - 2x)A$, $b_2 = (1 - 2x)B$, $b_3 = (1 - 2x)C$, $b_4 = (1 - 2x)D$.

Without loss of generality we can take that $A \geq B, C, D$ and $C \geq D$. There are three cases to be considered regarding how B is positioned to C, D:

(1) If $B \geq C$, then $A \geq B \geq C \geq D$. Since $x \in [0, 1/2]$, i.e., x, $1 - 2x \geq 0$, it is obvious that $b_1 \geq b_2 \geq b_3 \geq b_4$ and $\sum_{i=1}^{j} a_i \geq \sum_{i=1}^{j} b_i$, for $j = 1, 2, 3, 4$. So now the sequences a_1, a_2, a_3, a_4 and b_1, b_2, b_3, b_4 satisfy the conditions for the majorizing inequality.

Similarly to case (1) the orderings of a's and b's for the other two cases are:

(2) if $C \geq B \geq D$, then $A \geq C \geq B \geq D$, and a_1, a_3, a_2, a_4 and b_1, b_3, b_2, b_4;

(3) if $D \geq B$, then $A \geq C \geq D \geq B$, and a_1, a_3, a_4, a_2 and b_1, b_3, b_4, b_2;

and they satisfy the conditions for the majorizing inequality. □

Proof. (of the Theorem 1.1)
By Theorem 2.1 we have that the function $g(i,j,k,l)$ is non-negative for any positive integers i,j,k,l and any $\lambda \in [0, \frac{1}{2}]$. By Lemma 1.1, the function $f(i,j)$ is also non-negative for $\lambda \in [0, \frac{1}{2}] \subset [0,1]$. Since f and g are non-negative for $\lambda \in [0, \frac{1}{2}]$ we have ${}^{\lambda}M_2/m - {}^{\lambda}M_1/n \geq 0$ i.e., ${}^{\lambda}M_1/n \leq {}^{\lambda} M_2/m$. This completes the proof. □

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