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Comparing Zagreb Indices for Almost All Graphs

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Abstract

It was conjectured in literature that the inequality $\frac{M_1(G)}{n} \leq \frac{M_2(G)}{m}$ holds for all simple graphs, where $M_1(G)$ and $M_2(G)$ are the first and the second Zagreb index. By further research it was proven that the inequality holds for several graph classes such as chemical graphs, trees, unicyclic graphs and subdivided graphs, but that generally it does not hold since counter examples have been established in several other graph classes. So, the conjecture generally does not hold. Given the behavior of graphs satisfying the conjecture to some general graph operations it was further conjectured that the inequality might hold for almost all simple graphs. In this paper we will prove that this conjecture is true, by proving that the probability of a random graph G on n vertices to satisfy the inequality tends to 1 as n tends to infinity.

1 Introduction

For a simple graph $G = (V, E)$ having $n = |V|$ vertices and $m = |E|$ edges first Zagreb index $M_1(G)$ and second Zagreb index $M_2(G)$ are defined as

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

where $d_G(u)$ denotes the degree of vertex $u \in V$. These indices were introduced in [4], while the study of their chemical importance and mathematical properties is given in [1], [3], [5], [10], [13]. In [6] Hansen and Vukičević noted that for general graphs, the order of magnitude of M_1 is $O(n^3)$ while the order of magnitude of M_2 is $O(n^4)$ and that, therefore, it might be useful to compare M_1/n and M_2/m instead of comparing M_1 and M_2. They did some testing using AGX system ([2]) which led them to the following conjecture.

Conjecture 1 (posed in [6]) *For all simple connected graphs G it holds that*

$$\frac{M_1(G)}{n} \leq \frac{M_2(G)}{m}$$

and the bound is tight for complete graphs.

This turned out to be a very interesting conjecture, because it was proved that it is true for some well known graph classes such as chemical graphs ([6]), trees ([15]), unicyclic graphs ([8]) and subdivided graphs ([7]), while generally it does not hold since counter examples have been established in several other graph classes such as bicyclic graphs ([7], [14]) and graphs with large stars attached ([11]). Since the conjecture generated a lot of scientific research, a survey on the development of this conjecture was made in 2011 (see [9]). Still, the problem of characterizing graphs satisfying Conjecture 1 remained unsolved.

In [12] Stevanović made some further progress on the conjecture by proving that the set of graphs satisfying Conjecture 1 is closed under arbitrary NEPS graph operation, while the set of the counterexamples to Conjecture 1 is closed under the direct product of graphs only. Since NEPS graph operation is much more general than the direct product of graphs, this led Stevanović to conjecture in the conclusion of his paper the possibility that Conjecture 1 may be valid for the majority of graphs, perhaps even for almost all graphs. In this paper we will prove that Stevanović was right in conjecturing so, because (as we will prove) the probability that a random graph G on n vertices satisfies the Conjecture 1 tends to 1 as n tends to infinity.

2 Main results

Let Ω_n be the set of all simple graphs on n vertices and let the power set $\mathcal{P}(\Omega_n)$ be it's sigma algebra. Let $G \in \Omega_n$ be a graph on n vertices. For a vertex $u \in V$ of graph G we define x_u as

$$x_u = d_G(u) - \frac{n-1}{2}$$

where $d_G(u)$ denotes the degree of vertex u. Now, for a random graph $G \in \Omega_n$ with n vertices and m edges we define the following properties:

A_1) G is connected;

A_2) the inequality $\left|m - \frac{1}{2}\binom{n}{2}\right| \leq n^{1.1}$ holds for G;

A_3) the inequality $\sum_{u \in V} x_u^2 \geq n^{1.8}$ holds for G;

A_4) for every vertex $u \in V$ it holds that $|x_u| \leq n^{0.6}$;

A_5) for every vertex $u \in V$ it holds that $\left|\sum_{v, uv \in E} x_v\right| \leq n^{1.1}$.

In the context of sigma algebra $\mathcal{P}(\Omega_n)$ we can say that the set $A_i \in \mathcal{P}(\Omega_n)$ (for $i = 1, \ldots, 5$) consists of graphs $G \in \Omega_n$ which have property A_i. The following lemma gives us asymptotic probabilities of the events A_i^c, where A_i^c denotes the complement of A_i, and it is the collection of the results of several auxiliary lemmas which will be proved in the next section (the proofs are a bit lengthy and technical).

Lemma 2 *For every $i = 1, \ldots, 5$ it holds that*

$$\lim_{n \to \infty} P(A_i^c) = 0.$$

Proof. This lemma is direct consequence of Lemmas 8, 9, 10, 11 and 12 stated and proved in the next section. ■

Now, we can proceed to our main results.

Theorem 3 *Probability that random simple graph $G \in \Omega_n$ satisfies properties A_1, A_2, A_3, A_4 and A_5 tends to 1 as n tends to infinity.*

Proof. We want to establish probability of an event $A = A_1 \cap A_2 \cap A_3 \cap A_4 \cap A_5 \in \mathcal{P}(\Omega_n)$. Note that

$$P(A) = 1 - P(A^c) = 1 - P(A_1^c \cup A_2^c \cup A_3^c \cup A_4^c \cup A_5^c) \geq$$
$$\geq 1 - P(A_1^c) - P(A_2^c) - P(A_3^c) - P(A_4^c) - P(A_5^c).$$

From Lemma 2 it follows that

$$\lim_{n\to\infty} P(A) = 1 - \sum\nolimits_{i=1}^{5} \lim_{n\to\infty} P(A_i^c) = 1$$

which proves the theorem. ■

Theorem 4 *For sufficiently large n it holds that every simple graph $G \in \Omega_n$ which satisfies properties A_1, A_2, A_3, A_4 and A_5 also satisfies the inequality*

$$\frac{M_1(G)}{n} \leq \frac{M_2(G)}{m}.$$

Proof. Let $G \in A = A_1 \cap A_2 \cap A_3 \cap A_4 \cap A_5 \in \mathcal{P}(\Omega_n)$ be a graph with n vertices and m edges. Note that for the graph G the inequality from the theorem statement is equivalent to

$$n \sum_{uv\in E} \left(\frac{n-1}{2} + x_u\right)\left(\frac{n-1}{2} + x_v\right) - m \sum_{u\in V} \left(\frac{n-1}{2} + x_u\right)^2 \geq 0,$$

which can be rewritten as

$$n\left(\frac{n-1}{2}\right) \sum_{uv\in E} (x_u + x_v) + n \sum_{uv\in E} x_u x_v - 2m \left(\frac{n-1}{2}\right) \sum_{u\in V} x_u - m \sum_{u\in V} x_u^2 \geq 0.$$

Now, note that the following equality holds

$$\sum_{uv\in E} (x_u + x_v) = \sum_{u\in V} d_G(u) x_u = \sum_{u\in V} \left(\frac{n-1}{2} + x_u\right) x_u = \frac{n-1}{2} \sum_{u\in V} x_u + \sum_{u\in V} x_u^2.$$

Therefore, the inequality is further equivalent to

$$(n-1)\left(\frac{1}{2}\binom{n}{2} - m\right) \sum_{u\in V} x_u + \left(\binom{n}{2} - m\right) \sum_{u\in V} x_u^2 + n \sum_{uv\in E} x_u x_v \geq 0.$$

Now, using the handshaking lemma we note that

$$\sum_{u\in V} x_u = \sum_{u\in V} \left(d_G(u) - \frac{n-1}{2}\right) = 2m - \frac{n(n-1)}{2} = 2m - \binom{n}{2},$$

which means that the inequality is further equivalent to

$$(n-1)\left(\frac{1}{2}\binom{n}{2} - m\right)\left(2m - \binom{n}{2}\right) + \left(\binom{n}{2} - m\right) \sum_{u\in V} x_u^2 + n \sum_{uv\in E} x_u x_v \geq 0.$$

We have finally transformed the inequality to the form which is fit for proving using the properties of graph G. Let us denote

$$f(G)=(n-1)\left(\frac{1}{2}\binom{n}{2}-m\right)\left(2m-\binom{n}{2}\right)+\left(\binom{n}{2}-m\right)\sum_{u\in V}x_u^2+n\sum_{uv\in E}x_ux_v.$$

Now, since $G\in A\subseteq A_2$ we have

$$\left|(n-1)\left(\frac{1}{2}\binom{n}{2}-m\right)\left(2m-\binom{n}{2}\right)\right|\leq n\cdot n^{1.1}\cdot 2n^{11}=2n^{3.2}.$$

Also, since $G\in A\subseteq A_4\cap A_5$ we have

$$\left|n\sum_{uv\in E}x_ux_v\right|=\left|\frac{n}{2}\sum_{u\in V}x_u\sum_{v,uv\in E}x_v\right|\leq\frac{n}{2}\cdot n\cdot n^{0.6}\cdot n^{1.1}=\frac{1}{2}n^{3.7}.$$

Finally, since $G\in A_2\cap A_3$ we have

$$\begin{aligned}\left(\binom{n}{2}-m\right)\sum_{u\in V}x_u^2&=\left(\frac{1}{2}\binom{n}{2}-\left(m-\frac{1}{2}\binom{n}{2}\right)\right)\sum_{u\in V}x_u^2\\&\geq\left(\frac{1}{2}\binom{n}{2}-n^{1.1}\right)n^{1.8}.\end{aligned}$$

Therefore, it holds that

$$f(G)\geq\left(\frac{1}{2}\binom{n}{2}-n^{1.1}\right)n^{1.8}-2n^{3.2}-\frac{1}{2}n^{3.7}=g(n).$$

Since $\lim_{n\to\infty}g(n)=+\infty$, it follows that for sufficiently large n the expression $g(n)$ is positive, which further implies $f(G)\geq 0$ which proves the theorem. ■

Now, we can state the theorem which is the main result of this paper.

Theorem 5 *Probability that random graph G on n vertices satisfies the inequality*

$$\frac{M_1(G)}{n}\leq\frac{M_2(G)}{m}$$

tends to 1 *as n tends to infinity.*

Proof. This theorem is direct consequence of Theorems 3 i 4. ■

3 Auxiliary lemmas

Now, we first want to state and prove two lemmas with properties which will be of use to us in proving the five lemmas which will follow (in which we will prove that the probability of property A_i not holding for $G\in\Omega_n$ tends to zero as n tends to infinity for each $i=1,\ldots,5$).

Lemma 6 *If* $0.5 < \alpha < 1$, *then there is sufficiently large* $N_0 \in \mathbb{N}$ *such that for every integer* $N \geq N_0$ *and for every* $0 < \varepsilon < 2\alpha - 1$ *it holds that*

$$\frac{1}{2^N}\binom{N}{\left\lfloor \frac{N}{2} - N^\alpha \right\rfloor} = \frac{1}{2^N}\binom{N}{\left\lceil \frac{N}{2} + N^\alpha \right\rceil} \leq \frac{1}{2^{N^\varepsilon}}.$$

Proof. Let us denote $N_1 = \left\lfloor \frac{N}{2} - N^\alpha \right\rfloor$ and $N_2 = \left\lceil \frac{N}{2} + N^\alpha \right\rceil$. We will prove the claim for N_1 and then the claim for N_2 follows from symmetry of binomial coefficients. Let us denote $K = \frac{N}{2} - \left\lfloor \frac{N}{2} - N^\alpha \right\rfloor$. Now, $N_1 = \frac{N}{2} - K$ and $N_2 = \frac{N}{2} + K$, therefore $N_1 + N_2 = N$. Let us define function $f(N) = \frac{N!}{\sqrt{2\pi N}(\frac{N}{e})^N}$. Note that $\lim_{N\to\infty} f(N) = 1$. Now we have

$$\begin{aligned}\frac{1}{2^N}\binom{N}{N_1} &= \frac{1}{2^N}\frac{N!}{N_1!N_2!} \\ &= \frac{f(N)}{f(N_1)f(N_2)}\frac{\sqrt{2\pi N}}{\sqrt{2\pi N_1}\sqrt{2\pi N_2}}\frac{1}{2^N}\frac{N^N}{N_1^{N_1}N_2^{N_2}}.\end{aligned}$$

If we define function $g(N) = (1 + \frac{1}{N})^N$, it further holds

$$\begin{aligned}\frac{1}{2^N}\frac{N^N}{N_1^{N_1}N_2^{N_2}} &= \frac{1}{2^N}\frac{N^N}{(\frac{N}{2} - K)^{\frac{N}{2}-K}(\frac{N}{2} + K)^{\frac{N}{2}+K}} \\ &= \frac{1}{2^N}\frac{(N^2)^{\frac{N}{2}}}{(\frac{N^2}{4} - K^2)^{\frac{N}{2}}}\frac{(\frac{N}{2} + K)^{-K}}{(\frac{N}{2} - K)^{-K}} \\ &= \left(g(\frac{N^2 - 4K^2}{4K^2})^{\frac{N}{N+2K}}g(\frac{N-2K}{2K})^{-2}\right)^{\frac{2K^2}{N-2K}}.\end{aligned}$$

Note that $\lim_{N\to\infty} g(N) = e > 2$ and $\lim_{N\to\infty}(\frac{2K^2}{N-2K} \cdot N^{-\varepsilon}) > 1$ for every $0 < \varepsilon < 2\alpha - 1$. Therefore, there exists sufficiently large N_0 such that for every $N \geq N_0$ it holds that

$$\frac{1}{2^N}\binom{N}{N_1} \leq \frac{1}{2^{N^\varepsilon}}$$

which proves the lemma. ■

Lemma 7 *There is sufficiently large* $N_0 \in \mathbb{N}$ *such that for every integer* $N \geq N_0$ *it holds that*

$$\sum_{k=a}^{b}\frac{1}{2^N}\binom{N}{k} \leq \frac{b-a+1}{\sqrt{N}}.$$

Proof. Since

$$\sum_{k=a}^{b}\frac{1}{2^N}\binom{N}{k} \leq (b-a+1)\frac{1}{2^N}\binom{N}{\lceil N/2 \rceil}$$

it is sufficient to prove that for sufficiently large N it holds that $\frac{1}{2^N}\binom{N}{\lceil N/2\rceil} \leq \frac{1}{\sqrt{N}}$. Note that for even N using Stirling formula we obtain

$$\lim_{N\to\infty} \frac{\sqrt{N}}{2^N}\binom{N}{\lceil N/2\rceil} = \lim_{n\to\infty} \frac{\sqrt{N}}{2^N}\frac{\sqrt{2\pi N}(Ne^{-1})^N}{\left(\sqrt{2\pi\frac{N}{2}}(\frac{N}{2}e^{-1})^{\frac{N}{2}}\right)^2} = \sqrt{\frac{2}{\pi}} < 1.$$

The proof for odd n is similar, so the lemma is proved. ∎

Lemma 8 *It holds that* $\lim_{n\to\infty} P(A_1^c) = 0$.

Proof. Note that A_1^c consists of all graphs $G \in \Omega_n$ which are disconnected. Let B be the set of all graphs on n vertices in which at least one pair of vertices doesn't have common neighbor. Obviously, $A_1^c \subseteq B$. Note that $B = \cup_{u,v\in V} B_{u,v}$, where $B_{u,v}$ is the set of all graphs on n vertices in which pair of vertices $u, v \in V$ doesn't have common neighbor. It is obvious that $P(B_{u,v}) = (\frac{3}{4})^{n-2}$. Therefore, we have

$$P(A_1^c) \leq P(B) \leq \sum_{u,v\in V} P(B_{u,v}) = \binom{n}{2}\left(\frac{3}{4}\right)^{n-2} = f(n).$$

Now it follows that $\lim_{n\to\infty} P(A_1^c) \leq \lim_{n\to\infty} f(n) = 0$ and the lemma is proved. ∎

Lemma 9 *It holds that* $\lim_{n\to\infty} P(A_2^c) = 0$.

Proof. Note that A_2^c consists of all graphs $G \in \Omega_n$ in which the inequality $\left|m - \frac{1}{2}\binom{n}{2}\right| \leq n^{1.1}$ does not hold. Let us denote $N = \binom{n}{2}$. Now, we define

$$B_1 = \{G \in \Omega_n : m - \tfrac{N}{2} > n^{1.1}\},$$
$$B_2 = \{G \in \Omega_n : m - \tfrac{N}{2} < -n^{1.1}\}.$$

Obviously $A_2^c = B_1 \cup B_2$, where $B_1 \cap B_2 = \phi$. Therefore, it holds that $P(A_2^c) = P(B_1) + P(B_2)$. We have to prove that $\lim_{n\to\infty} P(B_i) = 0$ for $i = 1, 2$. Note that

$$P(B_1) = \frac{|B_1|}{|\Omega_n|} = \frac{1}{2^N}\sum\nolimits_{m=\lceil\frac{N}{2}+n^{1.1}\rceil}^{N}\tbinom{N}{m}$$
$$\leq \frac{N}{2^N}\max_{\lceil N/2+n^{1.1}\rceil<m\leq N}\tbinom{N}{m}$$
$$\leq \frac{N}{2^N}\binom{N}{\lceil N/2+n^{1.1}\rceil}$$

Since $N^{0.53} \leq (n^2)^{0.53} < n^{1.1}$, by Lemma 6 have

$$\lim_{n\to\infty} P(B_1) \leq \lim_{N\to\infty}\frac{N}{2^{N^{0.05}}} = 0.$$

The proof for $\lim_{n\to\infty} P(B_2) = 0$ is completely analogous, so the lemma is proved. ∎

Lemma 10 *It holds that* $\lim_{n\to\infty} P(A_3^c) = 0$.

Proof. Note that A_3 consists of all graphs $G \in \Omega_n$ in which the inequality $\sum_{u\in V} x_u^2 \geq n^{1.8}$ holds. Let us define B to be the set of all graphs $G \in \Omega_n$ in which for at least $\lceil n^{0.95} \rceil$ vertices $u \in V$ it holds that $|x_u| \geq n^{0.45}$. Note that for $G \in B$ it then holds that

$$\sum_{u\in V} x_u^2 \geq \lceil n^{0.95} \rceil (n^{0.45})^2 \geq n^{1.85}.$$

Therefore $B \subseteq A_3$, which implies $A_3^c \subseteq B^c$, which further implies that it is sufficient to prove that $\lim_{n\to\infty} P(B^c) = 0$. Note that B^c consists of all graphs $G \in \Omega_n$ in which for at most $\lceil n^{0.95} \rceil - 1$ vertices $u \in V$ it holds that $|x_u| \geq n^{0.45}$.

Now, for a graph $G \in \Omega_n$ with set of vertices $\{u_1, \dots, u_n\}$ let us define $d_G^-(u_i)$ to be the number of neighbors vertex u_i has in the set $\{u_1, \dots, u_{i-1}\}$, and let $d_G^+(u_i) = d_G(u_i) - d_G^-(u_i)$. For each $i = 1, \dots, n$ we further define B_i to consist of all graphs $G \in \Omega_n$ in which the equality $|x_{u_i}| < n^{0.45}$ holds. We want to establish the probability $P(B_i)$. For that purpose let us define events $D_{i,j} \in \mathcal{P}(\Omega_n)$ so that $D_{i,j}$ consists of those graphs $G \in \Omega_n$ in which $d_G^-(u_i) = j$ holds. Obviously, for every $i = 1, \dots, n$ it holds that

$$\Omega_n = D_{i,0} \cup D_{i,1} \cup \ldots \cup D_{i,i-1}$$

and $D_{i,j} \cap D_{i,k} = \phi$ for all $0 \leq j < k \leq i-1$. Therefore, it holds that

$$P(B_i) = P(B_i|D_{i,0})P(D_{i,0}) + P(B_i|D_{i,2})P(D_{i,2}) + \ldots + P(B_i|D_{i,i-1})P(D_{i,i-1}).$$

Let us establish $P(B_i|D_{i,j})$, i.e. probability that in a graph G vertex u_i for which $d_G(u_i) = j$ also satisfies $|x_{u_i}| < n^{0.45}$. Note that the inequality $|x_{u_i}| < n^{0.45}$ is equivalent to $\left|d_G(u_i) - \frac{n-1}{2}\right| < n^{0.45}$, which is further equivalent to

$$\frac{n-1}{2} - j - n^{0.45} < d_G^+(u_i) < \frac{n-1}{2} - j + n^{0.45}.$$

Therefore, by Lemma 7 we have

$$\begin{aligned} P(B_i|D_{i,j}) = \frac{|B_i|}{|D_{i,j}|} &= \frac{1}{2^{n-i}} \sum_{d=\left\lceil \frac{n-1}{2} - j - n^{0.45} \right\rceil}^{\left\lfloor \frac{n-1}{2} - j + n^{0.45} \right\rfloor} \binom{n-i}{d} \\ &\leq \left(\left\lfloor \frac{n-1}{2} - j + n^{0.45} \right\rfloor - \left\lceil \frac{n-1}{2} - j - n^{0.45} \right\rceil + 1 \right) \frac{1}{\sqrt{n-i}} \\ &\leq \frac{1 + 2n^{0.45}}{(n-i)^{0.5}}. \end{aligned}$$

Since $\lim_{n\to\infty} \frac{1+2n^{0.45}}{(n-i)^{0.5}} \cdot n^{0.04} = 0 < 1$ for $i \leq \lceil n^{0.99} \rceil$, we conclude that for sufficiently large n and $i \leq \lceil n^{0.99} \rceil$ it holds that $P(B_i|D_{i,j}) \leq n^{-0.04}$. Therefore, for sufficiently large n and $i \leq \lceil n^{0.99} \rceil$ we obtain

$$P(B_i) = \sum_{j=0}^{i-1} P(B_i|D_{i,j})P(D_{i,j}) \leq n^{-0.04} \sum_{j=0}^{i-1} P(D_{i,j}) = n^{-0.04}.$$

If we denote $p = 1 - n^{-0.04}$, this means that for $i \leq \lceil n^{0.99} \rceil$ the probability of vertex u_i to have $|x_u| \geq n^{0.45}$ is at least p. Let us define event D to consist of all graphs $G \in \Omega$ in which for at most $\lceil n^{0.95} \rceil - 1$ vertices from $\{u_1, \ldots, u_{\lceil n^{0.99} \rceil}\}$ it holds that $|x_u| \geq n^{0.45}$. Therefore, for sufficiently large n the probability $P(D)$ is smaller than the probability $P(B(\lceil n^{0.99} \rceil, p) < \lceil n^{0.95} \rceil)$ where $B(\lceil n^{0.99} \rceil, p)$ is binomial distribution. Note that $B^c \subseteq D$ which implies $P(B^c) \leq P(D)$. Therefore,

$$\begin{aligned}
\lim_{n\to\infty} P(B^c) &\leq \lim_{n\to\infty} P(D) \\
&\leq \lim_{n\to\infty} P(B(\lceil n^{0.99} \rceil, p) < \lceil n^{0.95} \rceil) \\
&\leq \lim_{n\to\infty} P(B(\lceil n^{0.99} \rceil, \frac{1}{2}) < \lceil n^{0.95} \rceil) \\
&\leq \lim_{n\to\infty} \sum_{k=0}^{\lceil n^{0.95} \rceil} \binom{\lceil n^{0.99} \rceil}{k} \left(\frac{1}{2}\right)^{\lceil n^{0.99} \rceil} \\
&\leq \lim_{n\to\infty} \frac{n}{2^{\lceil n^{0.99} \rceil}} \max_{0 \leq k \leq \lceil n^{0.95} \rceil} \binom{\lceil n^{0.99} \rceil}{k}.
\end{aligned}$$

Since for sufficiently large n it holds that

$$\lceil n^{0.95} \rceil \leq \left\lfloor \lceil n^{0.99} \rceil / 2 - \lceil n^{0.99} \rceil^{0.53} \right\rfloor$$

we further have

$$\lim_{n\to\infty} P(B^c) \leq \lim_{n\to\infty} \frac{n}{2^{\lceil n^{0.99} \rceil}} \binom{\lceil n^{0.99} \rceil}{\left\lfloor \lceil n^{0.99} \rceil / 2 - \lceil n^{0.99} \rceil^{0.53} \right\rfloor}.$$

Now by Lemma 6 we obtain

$$\lim_{n\to\infty} P(B^c) \leq \lim_{n\to\infty} \frac{n}{2^{\lceil n^{0.99} \rceil^{0.05}}} = 0.$$

which proves the lemma. ■

Lemma 11 *It holds that* $\lim_{n\to\infty} P(A_4^c) = 0$.

Proof. Note that A_4^c consists of all graphs $G \in \Omega_n$ in which for at least one vertex $u \in V$ it holds that $|x_u| > n^{0.6}$. Since $|x_u| > n^{0.6}$ is equivalent to $\left|d_G(u) - \frac{n-1}{2}\right| > n^{0.6}$, let us define

$$B_1 = \{G \in \Omega_n : (\exists u \in V)(d_G(u) > \tfrac{n-1}{2} + n^{0.6})\}$$
$$B_2 = \{G \in \Omega_n : (\exists u \in V)(d_G(u) < \frac{n-1}{2} - n^{0.6})\}$$

Obviously, it holds that $A_4^c = B_1 \cup B_2$. Therefore,

$$P(A_4^c) = P(B_1 \cup B_2) \leq P(B_1) + P(B_2).$$

Note that

$$\begin{aligned}
\lim_{n\to\infty} P(B_1) &= \lim_{n\to\infty} \frac{\binom{n}{1}}{2^{n-1}} \sum_{d=\lceil \frac{n-1}{2} + n^{0.6}\rceil}^{n-1} \binom{n-1}{d} \\
&\leq \lim_{n\to\infty} \frac{n^2}{2^{n-1}} \max_{\lceil \frac{n-1}{2} + n^{0.6}\rceil \leq d \leq n-1} \binom{n-1}{d} \\
&= \lim_{n\to\infty} \frac{n^2}{2^{n-1}} \binom{n-1}{\lceil \frac{n-1}{2} + n^{0.6}\rceil} \leq \{n^{0.6} < (n-1)^{0.53}\} \\
&\leq \lim_{n\to\infty} \frac{n^2}{2^{n-1}} \binom{n-1}{\lceil \frac{n-1}{2} + (n-1)^{0.53}\rceil}.
\end{aligned}$$

Now by Lemma 6 we obtain that

$$\lim_{n\to\infty} P(B_1) \leq \lim_{n\to\infty} \frac{n^2}{2^{(n-1)^{0.05}}} = 0.$$

Completely analogously one can prove that $\lim_{n\to\infty} P(B_2) = 0$ and the lemma is proved. ∎

Lemma 12 *It holds that* $\lim_{n\to\infty} P(A_5^c) = 0$.

Proof. Note that A_5^c consists of all graphs $G \in \Omega_n$ in which for at least one vertex $u \in V$ it holds that $\left|\sum_{v,uv\in E} x_v\right| > n^{1.1}$. Let us define

$$B_1 = \{G \in \Omega_n : (\exists u \in V)(\textstyle\sum_{v,uv\in E} x_v > n^{1.1})\},$$
$$B_2 = \{G \in \Omega_n : (\exists u \in V)(\textstyle\sum_{v,uv\in E} x_v < -n^{1.1})\}.$$

Note that $A_5^c = B_1 \cup B_2$, which implies that

$$P(A_5^c) = P(B_1 \cup B_2) \leq P(B_1) + P(B_2).$$

Let us first prove that $\lim_{n\to\infty} P(B_i) = 0$. For $u \in \{u_1, \ldots, u_n\}$ fixed, let us now define $B_{1,u} = \{G \in \Omega_n : \sum_{v,uv\in E} x_v > n^{1.1}\}$. Obviously, it holds that

$$B_1 = \bigcup_{u\in V} B_{1,u}$$

which implies

$$P(B_1) \le \sum_{u\in V} P(B_{1,u}).$$

We want to establish the upper bound on $P(B_{1,u})$ which does not depend on u, but only on n. For that purpose, let $v_1, \ldots, v_k$ be the neighbors of u in $G \in B_{1,u}$ and let $v_{k+1}, \ldots, v_{n-1}$ be the remaining vertices in G. If we define $\delta_{ij} = 1$ when $u_i u_j \in E$, while $\delta_{ij} = 0$ otherwise, note that $\sum_{v,uv\in E} x_v > n^{1.1}$ is equivalent to

$$2\left(\sum_{1\le i<j\le k} \delta_{ij} - \frac{1}{2}\binom{k}{2}\right) + \left(\sum_{1\le i\le k<j\le n-1} \delta_{ij} + \frac{k(n-k)}{2}\right) + k > n^{1.1}.$$

Let us now define

$$\begin{aligned} D_{1,u} &= \{G \in \Omega_n : \textstyle\sum_{1\le i<j\le k} \delta_{ij} - \frac{1}{2}\binom{k}{2} > n^{1.09}\}, \\ D_{2,u} &= \{G \in \Omega_n : \textstyle\sum_{1\le i\le k<j\le n-1} \delta_{ij} + \frac{k(n-k)}{2} > n^{1.09}\}. \end{aligned}$$

Note that for sufficiently large n it holds that $D_{1,u}^c \cap D_{2,u}^c \subseteq B_{1,u}^c$, which implies $B_{1,u} \subseteq D_{1,u} \cup D_{2,u}$, which further implies $P(B_{1,u}) \le P(D_{1,u}) + P(D_{2,u})$. Let us define S_u^k as the set of all graphs $G \in \Omega_n$ for which $d_G(u) = k$. Obviously, it holds that

$$\Omega_n = S_u^0 \cup S_u^1 \cup \ldots \cup S_u^{n-1}$$

while $S_u^k \cap S_u^j = \phi$ for $0 \le k < j \le n-1$. Therefore,

$$P(D_{i,u}) = P(D_{i,u}|S_u^0)P(S_u^0) + P(D_{i,u}|S_u^1)P(S_u^1) + \ldots + P(D_{i,u}|S_u^{n-1})P(S_u^{n-1}).$$

Let us first bound $P(D_{1,u})$ from above. Note that

$$\begin{aligned} P(D_{1,u}|S_u^k) &= 2^{-\binom{k}{2}} \sum_{p=\lceil \frac{1}{2}\binom{k}{2} + n^{1.09}\rceil}^{\binom{k}{2}} \binom{\binom{k}{2}}{p} \\ &\le \binom{k}{2} 2^{-\binom{k}{2}} \binom{\binom{k}{2}}{\lceil \frac{1}{2}\binom{k}{2} + n^{1.09}\rceil}. \end{aligned}$$

If $k < n^{0.54}$, then it holds that $\frac{1}{2}\binom{k}{2} \leq k^2 < n^{1.09}$, which implies that $P(D_{1,u}|S_u^k)$ is empty sum and therefore equal to zero. If on the other hand $k \geq n^{0.54}$, then $k \to \infty$ as $n \to \infty$ and it holds that

$$\binom{k}{2}^{0.53} \leq (n^2)^{0.53} \leq n^{1.09}.$$

Therefore, by Lemma 6 for sufficiently large $\binom{k}{2}$ it holds that

$$P(D_{1,u}|S_u^k) \leq \binom{k}{2} 2^{-\binom{k}{2}^{0.05}} \leq \{k \geq n^{0.54} \Rightarrow \binom{k}{2} \geq n\} \leq n \cdot 2^{-n^{0.05}}.$$

Now we have the following bound

$$P(D_{1,u}) = \sum_{k=0}^{n-1} P(D_{1,u}|S_u^k) P(S_u^k) \leq n \cdot 2^{-n^{0.05}} \sum_{k=0}^{n-1} P(S_u^k) = n \cdot 2^{-n^{0.05}}.$$

Let us now bound $P(D_{2,u})$ from above. Note that

$$\begin{aligned} p(D_{2,u}|S_u^k) &= \frac{1}{2^{k(n-k)}} \sum\nolimits_{p=\lceil \frac{1}{2}k(n-k)+n^{1.09} \rceil}^{k(n-k)} \binom{k(n-k)}{p} \\ &\leq \frac{k(n-k)}{2^{k(n-k)}} \binom{k(n-k)}{\lceil \frac{1}{2}k(n-k) + n^{1.09} \rceil}. \end{aligned}$$

If $k \leq n^{0.08}$, then $k(n-k) \leq kn < n^{1.09}$, which implies that $P(D_{2,u}|S_u^k)$ is empty sum and therefore equal to zero. If on the other hand $k > n^{0.08}$, then $k \to \infty$ as $n \to \infty$ and it holds that

$$(k(n-k))^{0.53} \leq (n^2)^{0.53} \leq n^{1.06} < n^{1.09}.$$

Therefore, by Lemma 6 for sufficiently large $k(n-k)$ it holds that

$$p(D_{2,u}|S_u^k) = k(n-k) \cdot 2^{-(k(n-k))^{0.05}} \leq \{k(n-k) > n\} \leq n \cdot 2^{-n^{0.05}},$$

which means we have the following bound

$$\begin{aligned} P(D_{2,u}) &= \sum_{k=0}^{n-1} P(D_{2,u}|S_u^k) P(S_u^k) \\ &\leq n \cdot 2^{-n^{0.05}} \sum_{k=0}^{n-1} P(S_u^k) = n \cdot 2^{-n^{0.05}}. \end{aligned}$$

Now for sufficiently large n we have

$$P(B_{1,u}) \leq P(D_{1,u}) + P(D_{2,u}) \leq 2n \cdot 2^{-n^{0.05}},$$

which further implies

$$P(B_1) \leq \sum_{u \in V} P(B_{1,u}) \leq \sum_{u \in V} 2n \cdot 2^{-n^{0.05}} = 2n^2 \cdot 2^{-n^{0.05}} = f(n).$$

Therefore, $\lim_{n\to\infty} P(B_1) \le \lim_{n\to\infty} f(n) = 0$. The proof that $\lim_{n\to\infty} P(B_2) = 0$ is completely analogous, so the lemma is proved. ■

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References

[1] V. Andova, S. Bogoev, D. Dimitrov, M. Pilipczuk, R. Škrekovski, On the Zagreb index inequality of graphs with prescribed vertex degrees, *Discr. Appl. Math.* **159** (2011) 852–858.

[2] M. Aouchiche, J. M. Bonnefoy, A. Fidahoussen, G. Caporossi, P. Hansen, L. Hiesse, J. Lacheré, A. Monhait, Variable neighborhood search for extremal graphs. 14. The AutoGraphiX 2 system, in: L. Liberti, N. Maculan (Eds.), *Global Optimization: From Theory to Implementation*, Springer, New York, 2006, pp. 281–310.

[3] G.H. Fath–Tabar, Old and new Zagreb index, *MATCH Commun. Math. Comput. Chem.* **65** (2011) 79–84.

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

[5] I. Gutman, K. C. Das, The first Zagreb index 30 years after, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 83–92.

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

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

[8] B. Liu, On a conjecture about comparing Zagreb indices, in: I. Gutman, B. Furtula (Eds.), *Recent Results in the Theory of Randić index*, Univ. Kragujevac, Kragujevac, 2008, pp. 205–209.

[9] B. Liu, Z. You, A survey on comparing Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **65** (2011) 581–593.

[10] S. Nikolić, G. Kovačević, A. Miličević, N. Trinajstić, The Zagreb indices 30 years after, *Croat. Chem. Acta* **73** (2003) 113–124.

[11] S. Stevanović, On a relation between the Zagreb indices, *Croat. Chem. Acta.* **84** (2011) 17–19.

[12] D. Stevanović, Comparing the Zagreb indices of the NEPS of graphs, *Appl. Math. Comput.* **219** (2012) 1082–1086.

[13] G. Su, L. Xiong, L. Xu, B. Ma, On the maximum and minimum rst reformulated Zagreb index of graphs with connectivity at most k, *Filomat* **25** (2011) 75–83.

[14] L. Sun, S. Wei, Comparing the Zagreb indices for connected bicyclic graphs, *MATCH Commun. Math. Comput. Chem.* **62** (2009) 699–714.

[15] D. Vukičević, A. Graovac, Comparing Zagreb M_1 and M_2 indices for acyclic molecules, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 587–590.