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Research Article

Modified Total Sigma-Irregularity in Chemical Graphs

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Abstract

The total σ-irregularity is a graph irregularity measure defined for a graph G as $\sigma_t(G) = \sum_{\{u,v\}\subseteq V(G)}(d_G(u) - d_G(v))^2$, where $d_G(w)$ denotes the degree of a vertex w in G. Graphs that maximize σ_t-irregularity consist of vertices having only two distinct degrees. In some sense, one might expect that in graphs with maximal irregularity all possible vertex degrees should occur - such graphs are known as antiregular. Motivated by this discrepancy, in our previous paper [*Appl. Math. Comput.* **490** (2025) #129199], we introduced a modified version of σ_t, which is defined by $\sigma_t^{f(n)}(G) = \sum_{\{u,v\}\subseteq V(G)} |d_G(u) - d_G(v)|^{f(n)}$, where $f(n) > 0$ is a positive real function depending on $n = |V(G)|$. That study examined under which conditions the modified invariant attains its maximum for antiregular graphs and conjectured that antiregular graphs maximize this modification whenever $f(n)$ is a constant in the interval $(0, 1)$. In the present work, this conjecture is disproved for chemical graphs. More precisely, we construct counterexamples showing that the conjectured extremal graphs fail to maximize the invariant in several cases. Furthermore, we provide a detailed analysis of the structural properties of degree sequences underlying these counterexamples and identify the correct extremal behavior in the considered setting.

Keywords: irregularity; total σ-irregularity; antiregular graphs; chemical graphs.

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1. Introduction and Preliminaries

Graph irregularity measures quantify deviations from regularity and have been extensively studied in graph theory as well as in applications to chemistry and network analysis [5, 10, 11, 18, 19]. A graph is called *antiregular* if all its vertices have distinct degrees except for exactly one pair of vertices having the same degree.

The *imbalance* of an edge $e = uv \in E$ is defined as $\mathrm{imb}(e) = |d_G(u) - d_G(v)|$. In [3], Albertson defined the *irregularity* of G as the sum of imbalances of all edges of the graph, i.e.,

$$\mathrm{irr}(G) = \sum_{e\in E(G)} \mathrm{imb}(e) = \sum_{uv\in E(G)} |d_G(u) - d_G(v)|. \tag{1}$$

Further insights into the Albertson irregularity index are available in [1, 14].

An alternative to the Albertson irregularity index, aimed at avoiding the absolute value computation, led to the introduction of the irregularity index $\sigma(G)$ in [13], defined as

$$\sigma(G) = \sum_{uv\in E(G)} (d_G(u) - d_G(v))^2.$$

Graphs with maximal σ-irregularity were characterized in [2], where lower bounds on σ-irregularity were also established. The inverse problem - determining the existence of a graph with σ-irregularity equal to a given non-negative integer - was addressed in [13]. Réti [17] further compared σ-irregularity with various other irregularity measures across specific graph classes. In [4], connected k-cyclic graphs with maximal σ-irregularity were determined.

If a sequence $S = (d_1, d_2, \ldots, d_n)$ corresponds to the degrees of vertices in some graph, it is called *graphical*. When arranged in non-increasing order, $d_1 \geq d_2 \geq \cdots \geq d_n$, it is referred to as a *degree sequence*. We use the following notation for degree sequences:

$$S = (1^{a_1}, 2^{a_2}, \ldots),$$

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where a_1 is the number of vertices of degree 1, a_2 the number of vertices of degree 2, and so on. The characterization of extremal graphs with respect to σ-irregularity for a given degree sequence was recently undertaken in [6].

A connected graph with maximum degree at most 4 is commonly referred to as a *chemical graph*, while a non-cyclic chemical graph is denoted as a *chemical tree*. Chemical graphs are of fundamental importance in mathematical chemistry, as they naturally represent molecular structures where vertices correspond to atoms and edges to chemical bonds. In [2], it was shown that among chemical trees, the path graph exhibits the smallest σ-irregularity. Furthermore, [16] characterizes chemical trees with maximal σ-irregularity. Trees with maximal σ-irregularity and maximum degree 5 were described in [7].

Graphs sharing the same degree sequence do not necessarily have the same σ-irregularity (see Figure 1 in [8] for an example). To address this, a variant of σ-irregularity invariant with respect to a given degree sequence was introduced in [8]. Earlier, a similar concept - motivated differently - had been independently proposed by Réti [17]. It is known as the *total σ-irregularity* and is defined as

$$\sigma_t(G) = \sum_{\{u,v\}\subseteq V(G)} \left(d_G(u) - d_G(v)\right)^2 .$$

The study [8] provided the first examination of σ_t, deriving the relation $\sigma_t(G) = nM_1(G) - 4m^2$ for simple connected graphs, thereby offering a quantitative interpretation of this measure. That work also analyzed σ_t in trees, identifying the star as the tree with the largest σ_t and the path as the one with the smallest σ_t.

A subsequent investigation [12] demonstrated that σ_t coincides with the degree variance of a graph. This connection enabled the characterization of irregular graphs maximizing σ_t-irregularity. Among all connected graphs on n vertices, the split graphs $S_{\lceil n/4\rceil,\lfloor 3n/4\rfloor}$ and $S_{\lfloor n/4\rfloor,\lceil 3n/4\rceil}$ were identified as extremal, while within the class of complete bipartite graphs on n vertices, the graphs $K_{\lfloor n(2-\sqrt{2})/4\rfloor,\lceil n(2+\sqrt{2})/4\rceil}$ and $K_{\lceil n(2-\sqrt{2})/4\rceil,\lfloor n(2+\sqrt{2})/4\rfloor}$ attain the highest values of the sigma total index.

Further contributions in [12] include several upper and lower bounds for σ_t-irregularity and explicit relationships between the graph energy $\mathcal{E}(G)$ and the sigma total index $\sigma_t(G)$. These relations also yield alternative proofs of two earlier results from [8]. Moreover, by applying Fiedler's characterization of the largest and second-smallest Laplacian eigenvalues, new connections between σ_t and the classical irregularity measure σ were obtained.

The graphs that maximize σ_t-irregularity are split graphs, i.e., graphs with few distinct degrees. Since one might expect that graphs with as many distinct degrees as possible should achieve maximal irregularity, this motivates the modified invariant

$$\sigma_t^{f(n)}(G) = \sum_{\{u,v\}\subseteq V(G)} |d_G(u) - d_G(v)|^{f(n)},$$

where $n = |V(G)|$ and $f(n) > 0$. In [15], the conditions under which the above modification attains its maximum in antiregular graphs were examined. That work also addressed general graphs, trees, and chemical graphs, and proposed several open problems and conjectures. Among other results, in [15] the following theorem concerning chemical graphs was established.

Theorem 1.1. *Let $n \geq 7$, $f(n) \leq \log_3\left(\frac{3n^2}{3n^2-8}\right)$, and let $(1^{a_1}, 2^{a_2}, 3^{a_3}, 4^{a_4})$ be a degree sequence of a chemical graph G with the maximum value of $\sigma_t^{f(n)}(G)$. Then:*

1. *If $n = 4k-1$, then $a_1 = a_3 = a_4 = k$ and $a_2 = k-1$;*
2. *If $n = 4k$, then $a_1 = a_2 = a_3 = a_4 = k$;*
3. *If $n = 4k+1$, then $a_1 = a_2 = a_3 = k$ and $a_4 = k+1$;*
4. *If $n = 4k+2$, then either $a_1 = a_3 = k$, $a_2 = a_4 = k+1$, or $a_1 = a_3 = k+1$, $a_2 = a_4 = k$.*

Motivated by these observations and empirical findings, the following conjecture was also proposed in [15].

Conjecture 1.1. *The same graphs as in Theorem 1.1 also maximize $\sigma_t^{f(n)}(G)$ when $f(n)$ is a constant in the interval $(0,1)$.*

The purpose of this paper is to show that this conjecture does not hold in general. We construct counterexamples demonstrating that the conjectured extremal graphs fail to maximize the invariant once the modification is applied. Our counterexamples rely on a detailed analysis of degree sequences with bounded maximum degree, leading to a general criterion for the graphicality of sequences of the form $(1^{a_1}, 2^{a_2}, 3^{a_3}, 4^{a_4})$, which plays a central role in our arguments.

2. Results

We consider chemical graphs, i.e., graphs whose maximum degree does not exceed 4. To simplify our calculations, we restrict ourselves to the case $n \equiv 0 \pmod 4$. By Theorem 1.1, for $n \geq 7$ and $f(n) \leq \log_3\left(\frac{3n^2}{3n^2-8}\right)$, the graphs on n vertices that maximize $\sigma_t^{f(n)}(G)$ have degree sequence $S_0 = (1^k, 2^k, 3^k, 4^k)$, where $k = n/4$.

In [15], it was conjectured that for any c in the interval $(0, 1)$, the graph G_0 with degree sequence S_0 attains the maximum value of σ_t^c. However, in the next proposition, we show that a graph G_k with degree sequence $S_k = (1^{2k}, 2^0, 3^0, 4^{2k})$ achieves a larger value of σ_t^c when c is close to 1.

In Proposition 2.1 we need a root q of equation $3^x - 2^x - 3 = 0$. Denote $r(x) = 3^x - 2^x - 3$. Since $r(x) < 0$ if $x \leq 0$, the root is positive. However, for positive x we have $r'(x) = 3^x \ln 3 - 2^x \ln 2 > 0$, and so $r(x)$ is increasing on $(0, \infty)$. Hence, it has at most one root and it turns out that its value is $q \doteq 1.65248$. Then $q - 1 \doteq 0.65248$.

Proposition 2.1. *Let q be the root of equation $3^q - 2^q - 3 = 0$.*

(a) If $c \in (0, q-1)$ then $\sigma_t^c(G_0) > \sigma_t^c(G_k)$;

(b) If $c = q - 1$ then $\sigma_t^c(G_0) = \sigma_t^c(G_k)$;

(c) If $c \in (q-1, 1)$ then $\sigma_t^c(G_0) < \sigma_t^c(G_k)$.

Proof. Observe that $\sigma_t^c(G_0) = 3k^2 \cdot 1 + 2k^2 \cdot 2^c + k^2 \cdot 3^c$ and $\sigma_t^c(G_k) = 0 \cdot 1 + 0 \cdot 2^c + 4k^2 \cdot 3^c$. Obviously

$$\sigma_t^0(G_0) = 6k^2 > 4k^2 = \sigma_t^0(G_k)$$
$$\sigma_t^1(G_0) = 10k^2 < 12k^2 = \sigma_t^1(G_k).$$

Since $\sigma_t^c(G_k) - \sigma_t^c(G_0) = k^2(3^{c+1} - 2^{c+1} - 3)$ is equal to 0 if $q = c + 1$ is the root of $3^q - 2^q - 3 = 0$, (since $3^q - 2^q - 3$ is monotonically increasing in q) we get the result. □

Proposition 2.1 shows that in some cases $\sigma_t^c(G_k) > \sigma_t^c(G_0)$. However, for every $c \in (0, 1)$, neither G_0 nor G_k maximizes σ_t^c when $n = 4k$ is big enough. To show this we first describe the class of possible extremal graphs.

For $n = 4$, it is straightforward to check that the star S_4 maximizes σ_t^c. Hence, in what follows, we restrict attention to $n \geq 8$.

The following proposition characterizes graphical sequences of degrees in $\{1, 2, 3, 4\}$ and will serve as a tool in the subsequent analysis.

Proposition 2.2. *Let $S = (1^{a_1}, 2^{a_2}, 3^{a_3}, 4^{a_4})$ be a sequence of nonnegative integers with $n = a_1 + a_2 + a_3 + a_4$, where $n \geq 8$. Then S is graphical if and only if $a_1 + a_3$ is even.*

Proof. *Necessity.* Suppose that S is graphical. Then the total degree sum

$$\sum_{i=1}^{n} d_i = a_1 + 2a_2 + 3a_3 + 4a_4 = (a_1 + a_3) + 2(a_2 + a_3 + 2a_4)$$

must be even. This implies that $a_1 + a_3$ is even, proving the necessity.

Sufficiency. Assume that $a_1 + a_3$ is even. By the Erdős–Gallai theorem [9], a non-increasing sequence $d_1 \geq \cdots \geq d_n$ is graphical if and only if

$$\sum_{i=1}^{k} d_i \leq k(k-1) + \sum_{i=k+1}^{n} \min(d_i, k) \quad \text{for all } k = 1, \ldots, n$$

and $\sum_{i=1}^{n} d_i$ is even. The total degree sum equals $(a_1 + a_3) + 2(a_2 + a_3 + 2a_4)$, so it is even by assumption. Hence, it remains to check the Erdős–Gallai inequalities.

For $k \geq 5$ we have $\sum_{i=1}^{k} d_i \leq 4k \leq k(k-1)$, so the Erdős–Gallai inequality is satisfied.

Observe that $\sum_{i=k+1}^{n} \min(d_i, k) \geq n - k$. Since for small values of $k = 1, 2, 3, 4$ we have

$$\sum_{i=1}^{k} d_i \leq 4k \leq k(k-1) + (9-k) \leq k(k-1) + \sum_{i=k+1}^{n} \min(d_i, k)$$

$g(x)$ x with equality only if $k = 3$ and when the degree sequence is $(1^6, 2^0, 3^0, 4^3)$, the Erdős–Gallai inequality is satisfied when $n \geq 9$.

For $n = 8$ the inequality $4k \le k(k-1) + (8-k)$ is not satisfied only if $k = 3$. So the Erdős–Gallai inequality is violated only for the sequence $(1^5, 2^0, 3^0, 4^3)$, which does not satisfy that $a_1 + a_3$ is even.

Thus, all Erdős–Gallai inequalities are satisfied. Together with the even total degree sum, we conclude that S is graphical. □

Having established a simple criterion for when a sequence is graphical, we can now analyze which of these sequences can belong to a chemical graph that maximizes σ_t^c.

Lemma 2.1. *Let c satisfy $0 \le c \le 1$ and let $n \equiv 0 \pmod 4$, $n \ge 8$. Let $S = (1^{a_1}, 2^{a_2}, 3^{a_3}, 4^{a_4})$ be the degree sequence of a chemical graph G on n vertices with the maximum value of σ_t^c. Then $a_1 = a_4$, $a_2 = a_3$ and $a_1 \ge a_2$.*

Proof. By Proposition 2.2, S is graphical if and only if $a_1 + a_3$ is even. By a sequence of changes on S we show that, if S does not satisfy the requirements from the statement, then there is a chemical graph G' with degree sequence S' such that $\sigma_t^c(G') > \sigma_t^c(G)$.

First observe that if a graph H has degree sequence $(1^{a_4}, 2^{a_3}, 3^{a_2}, 4^{a_1})$, then $\sigma_t^c(H) = \sigma_t^c(G)$. This observation reduces the number of cases needed to consider. In the cases below we first construct a sequence S' such that the sum of exponents on 1 and 3 is even. Then S' is graphical, so we denote by G' a graph with degree sequence S'. Further, we show that $\Delta > 0$, where $\Delta = \sigma_t^c(G') - \sigma_t^c(G)$. Observe that

$$\sigma_t^c(G) = (a_1a_2 + a_2a_3 + a_3a_4) + (a_1a_3 + a_2a_4)2^c + a_1a_4 3^c.$$

Case 1. $a_1 \le a_4 - 2$ and $a_2 \le a_3 - 2$. Let $S' = (1^{a_1+1}, 2^{a_2+1}, 3^{a_3-1}, 4^{a_4-1})$. Then

$$\begin{aligned}
\sigma_t^c(G') =& \big((a_1+1)(a_2+1) + (a_2+1)(a_3-1) + (a_3-1)(a_4-1)\big) + \big((a_1+1)(a_3-1) + (a_2+1)(a_4-1)\big)2^c + (a_1+1)(a_4-1)3^c\\
\Delta =& (a_1+a_2+1 + a_3-a_2-1 - a_3-a_4+1) + (a_3-a_1-1 + a_4-a_2-1)2^c + (a_4-a_1-1)3^c\\
=& (a_4 - a_1 - 1)(3^c + 2^c - 1) + (a_3 - a_2 - 1)2^c > 0
\end{aligned}$$

since both products are positive.

Case 2. $a_1 \le a_4 - 2$ and $a_3 \le a_2 - 2$. Let $S' = (1^{a_1+1}, 2^{a_2-1}, 3^{a_3+1}, 4^{a_4-1})$. Then

$$\begin{aligned}
\sigma_t^c(G') =& \big((a_1+1)(a_2-1) + (a_2-1)(a_3+1) + (a_3+1)(a_4-1)\big) + \big((a_1+1)(a_3+1) + (a_2-1)(a_4-1)\big)2^c + (a_1+1)(a_4-1)3^c\\
\Delta =& (a_2-a_1-1 + a_2-a_3-1 + a_4-a_3-1) + (a_1+a_3+1 - a_2-a_4+1)2^c + (a_4-a_1-1)3^c\\
=& (a_2 - a_3 - 1)(2 - 2^c) + (a_4 - a_1 - 1)(3^c - 2^c + 1) > 0.
\end{aligned}$$

Case 3. $a_1 = a_4$ and $a_2 < a_3$. Since $a_1 = a_4$ and both $a_1 + a_3$ and $a_1 + a_2 + a_3 + a_4$ are even, all a_1, a_2, a_3 and a_4 have the same parity. Thus a_3 differs from a_2 by an even number. But if $a_3 = a_2 + 2$, then $a_1 + a_2 + a_3 + a_4 \equiv 2 \pmod 4$, a contradiction. Hence $a_2 \le a_3 - 4$. Let $S' = (1^{a_1}, 2^{a_2+2}, 3^{a_3-2}, 4^{a_4})$. We have

$$\begin{aligned}
\sigma_t^c(G') =& \big(a_1(a_2+2) + (a_2+2)(a_3-2) + (a_3-2)a_4\big) + \big(a_1(a_3-2) + (a_2+2)a_4\big)2^c + a_1a_4 3^c\\
\Delta =& (2a_1 + 2a_3 - 2a_2 - 4 - 2a_4) + (-2a_1 + 2a_4)2^c\\
=& 2(a_4 - a_1)(2^c - 1) + 2(a_3 - a_2 - 2) > 0.
\end{aligned}$$

Case 4. $a_1 < a_4$ and $a_2 = a_3$. Then $a_1 \le a_4 - 4$ analogously as in Case 3. So let $S' = (1^{a_1+2}, 2^{a_2}, 3^{a_3}, 4^{a_4-2})$. We have

$$\begin{aligned}
\sigma_t^c(G') =& \big((a_1+2)a_2 + a_2a_3 + a_3(a_4-2)\big) + \big((a_1+2)a_3 + a_2(a_4-2)\big)2^c + (a_1+2)(a_4-2)3^c\\
\Delta =& (2a_2 - 2a_3) + (2a_3 - 2a_2)2^c + (2a_4 - 2a_1 - 4)3^c\\
=& 2(a_3 - a_2)(2^c - 1) + 2(a_4 - a_1 - 2)3^c > 0.
\end{aligned}$$

Case 5. $a_4 = a_1 + 1$ and $a_2 \le a_3 - 2$. Then $a_2 \le a_3 - 3$. So let $S' = (1^{a_1}, 2^{a_2+2}, 3^{a_3-2}, 4^{a_4})$. We have

$$\begin{aligned}
\sigma_t^c(G') =& \big(a_1(a_2+2) + (a_2+2)(a_3-2) + (a_3-2)a_4\big) + \big(a_1(a_3-2) + (a_2+2)a_4\big)2^c + a_1a_4 3^c\\
\Delta =& (2a_1 + 2a_3 - 2a_2 - 4 - 2a_4) + (2a_4 - 2a_1)2^c\\
=& 2(a_4 - a_1)(2^c - 1) + 2(a_3 - a_2 - 2) > 0.
\end{aligned}$$

Case 6. $a_4 = a_1 + 1$ and $a_3 \le a_2 - 2$. Then $a_3 \le a_2 - 3$. So let $S' = (1^{a_1}, 2^{a_2-2}, 3^{a_3+2}, 4^{a_4})$. We have

$$\begin{aligned}\sigma_t^c(G') =& \big(a_1(a_2-2) + (a_2-2)(a_3+2) + (a_3+2)a_4\big) + \big(a_1(a_3+2) + (a_2-2)a_4\big)2^c + a_1a_4 3^c\\ \Delta =& (-2a_1 + 2a_2 - 2a_3 - 4 + 2a_4) + (2a_1 - 2a_4)2^c\\ =& 2(a_4-a_1)(1-2^c) + 2(a_2-a_3-2)\\ =& 2(1-2^c) + 2(a_2-a_3-2) \ge 2(1-2^1) + 2(3-2) = 0\end{aligned}$$

with equality if and only if $c = 1$ and $a_3 = a_2 - 3$. However, if this happens then S' is exactly the sequence S in Case 9 below and as shown there, G' (and hence also G) does not achieve the maximum value of σ_t^c.

Case 7. $a_3 = a_2 + 1$ and $a_1 \le a_4 - 2$. Then $a_1 \le a_4 - 3$. So let $S' = (1^{a_1+2}, 2^{a_2}, 3^{a_3}, 4^{a_4-2})$. We have

$$\begin{aligned}\sigma_t^c(G') =& \big((a_1+2)a_2 + a_2a_3 + a_3(a_4-2)\big) + \big((a_1+2)a_3 + a_2(a_4-2)\big)2^c + (a_1+2)(a_4-2)3^c\\ \Delta =& (2a_2 - 2a_3) + (2a_3 - 2a_2)2^c + (2a_4 - 2a_1 - 4)3^c\\ =& 2(a_3-a_2)(2^c-1) + 2(a_4-a_1-2)3^c > 0.\end{aligned}$$

Case 8. $a_3 = a_2 + 1$ and $a_4 \le a_1 - 2$. Then $a_4 \le a_1 - 3$. So let $S' = (1^{a_1-2}, 2^{a_2}, 3^{a_3}, 4^{a_4+2})$. We have

$$\begin{aligned}\sigma_t^c(G') =& \big((a_1-2)a_2 + a_2a_3 + a_3(a_4+2)\big) + \big((a_1-2)a_3 + a_2(a_4+2)\big)2^c + (a_1-2)(a_4+2)3^c\\ \Delta =& (-2a_2 + 2a_3) + (-2a_3 + 2a_2)2^c + (2a_1 - 2a_4 - 4)3^c\\ =& 2(a_3-a_2)(1-2^c+3^c) + 2(a_1-a_4-3)3^c > 0,\end{aligned}$$

where for the last expression we used that $2(a_3-a_2)3^c = 2\cdot 1\cdot 3^c$, and while the second product is nonnegative, the first one is positive.

By Cases 1–8, it remains to consider the situation when $|a_4 - a_1| \le 1$ and $|a_3 - a_2| \le 1$.

Case 9. $a_4 = a_1 + 1$. Then $a_3 \ne a_2$. So either $a_3 = a_2 + 1$ or $a_3 = a_2 - 1$. But the latter case means that $a_1 + a_3 = a_1 + a_2 - 1$ is even since S is graphical. And since $a_1 + a_3 + a_2 + a_4 = (a_1 + a_2 - 1) + (a_1 + a_2 + 1)$, the sum of vertices cannot be $\equiv 0 \pmod 4$, a contradiction. So $a_3 = a_2 + 1$. Then $S = (1^{a_1}, 2^{a_2}, 3^{a_2+1}, 4^{a_1+1})$ and

$$\sigma_t^c(G) = \big(a_1a_2 + a_2(a_2+1) + (a_2+1)(a_1+1)\big) + \big(a_1(a_2+1) + +a_2(a_1+1)\big)2^c + a_1(a_1+1)3^c.$$

Now consider graphs G' and G'' with graphical sequences $S' = (1^{a_1}, 2^{a_2+1}, 3^{a_2+1}, 4^{a_1})$ and $S'' = (1^{a_1+1}, 2^{a_2}, 3^{a_2}, 4^{a_1+1})$, respectively. Then

$$\begin{aligned}\sigma_t^c(G') =& \big(a_1(a_2+1) + (a_2+1)(a_2+1) + (a_2+1)a_1)\big) + \big(a_1(a_2+1) + (a_2+1)a_1\big)2^c + a_1a_1 3^c\\ \sigma_t^c(G'') =& \big((a_1+1)a_2 + a_2a_2 + a_2(a_1+1)\big) + \big((a_1+1)a_2 + a_2(a_1+1)\big)2^c + (a_1+1)(a_1+1)3^c.\end{aligned}$$

Denote $\Delta' = \sigma_t^c(G') - \sigma_t^c(G)$ and $\Delta'' = \sigma_t^c(G'') - \sigma_t^c(G)$. We have

$$\begin{aligned}\Delta' =& (a_1 + a_2 + 1 - a_2 - 1) + (a_1 - a_2)2^c + (-a_1)3^c\\ \Delta'' =& (a_2 - a_2 - a_1 - 1) + (a_2 - a_1)2^c + (a_1+1)3^c.\end{aligned}$$

So $\Delta' + \Delta'' = -1 + 1\cdot 3^c \ge 0$, where equality holds only if $c = 0$. In all other cases either $\Delta' > 0$ or $\Delta'' > 0$ which means that either $\sigma_t^c(G') > \sigma_t^c(G)$ or $\sigma_t^c(G'') > \sigma_t^c(G)$. In the case $c = 0$ we have $\Delta' = a_1 - a_2$ and $\Delta'' = a_2 - a_1$ and if $a_1 \ne a_2$ we may conclude that G is not extremal. But the case $a_1 = a_2$ means that $n = a_1 + a_2 + a_2 + 1 + a_1 + 1 = 4a_1 + 2$ and so $n \not\equiv 0 \pmod 4$, a contradiction.

By Cases 1–9 we have $a_1 = a_4$ and $a_2 = a_3$. So it remains to solve the case when $a_1 < a_2$.

Case 10: $a_1 = a_4$, $a_2 = a_3$ and $a_1 < a_2$. Then $a_1 \le a_2 - 2$. Let $S' = (1^{a_1+1}, 2^{a_2-1}, 3^{a_2-1}, 4^{a_1+1})$. Then

$$\begin{aligned}\sigma_t^c(G) =& (a_1a_2 + a_2a_2 + a_2a_1) + (a_1a_2 + a_2a_1)2^c + a_1a_1 3^c\\ \sigma_t^c(G') =& \big((a_1+1)(a_2-1) + (a_2-1)(a_2-1) + (a_2-1)(a_1+1)\big) + \big((a_1+1)(a_2-1) + (a_2-1)(a_1+1)\big)2^c + (a_1+1)(a_1+1)3^c\\ \Delta =& (a_2 - a_1 - 1 - 2a_2 + 1 + a_2 - a_1 - 1) + (a_2 - a_1 - 1 + a_2 - a_1 - 1)2^c + (2a_1 + 1)3^c\\ =& (2a_1+1)(3^c-1) + 2(a_2-a_1-1)2^c > 0.\end{aligned}$$

Consequently, $a_1 = a_4$, $a_2 = a_3$ and $a_1 \ge a_2$. □

Let $0 \le a \le k$ and let $S_a = (1^{k+a}, 2^{k-a}, 3^{k-a}, 4^{k+a})$. Note that the sequence S_a is graphical since $a_1 + a_3 = k + a + k - a = 2k$ is even. Denote by G_a a graph with degree sequence S_a.

With the structure of potential extremal graphs established by the previous lemma, we can now determine precisely which degree sequence maximizes σ_t^c.

Theorem 2.1. *Let $c \in [0,1]$ and let $n = 4k$, where $k \ge 2$. Denote*

$$x_c = \frac{3^c - 1}{2 \cdot 2^c - 3^c + 1} k$$

and denote $a_c = Round(x_c)$.

(a) If $a_c - x_c = 0.5$ then both G_a and G_{a-1} maximize σ_t^c;

(b) If $|a_c - x_c| < 0.5$ then G_a maximizes σ_t^c.

Proof. Let $a \in [0,k] \cap \mathbb{N}$. Then

$$\begin{aligned}\sigma_t^c(G_a) =& \big((k+a)(k-a) + (k-a)(k-a) + (k-a)(k+a)\big) + \big((k+a)(k-a) + (k-a)(k+a)\big)2^c + (k+a)(k+a)3^c \\ =& (3k^2 - 2ka - a^2) + 2(k^2 - a^2)2^c + (k^2 + 2ka + a^2)3^c.\end{aligned}$$

Let $h(x) = (3k^2 - 2kx - x^2) + 2(k^2 - x^2)2^c + (k^2 + 2kx + x^2)3^c$ be a real-valued function defined on $[0,k]$. Then $\sigma_t^c(G_a) = h(a)$. The function $h(x)$ is quadratic and $h'(x) = (-2k - 2x) - 4x2^c + (2k + 2x)3^c$.

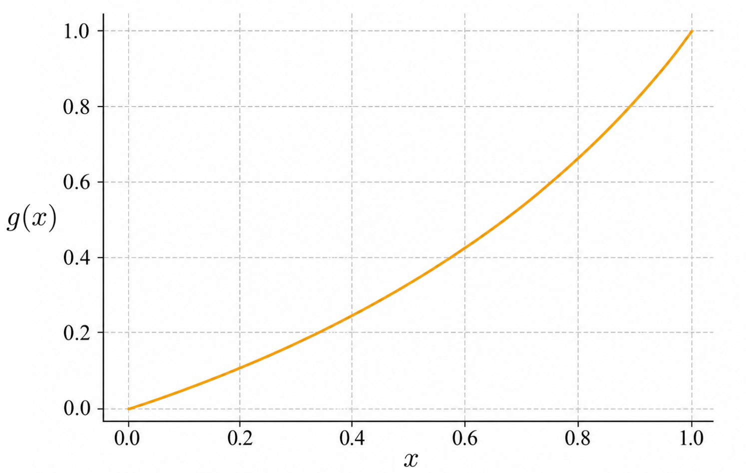

Figure 2.1: Plot of the function $g(x) = (3^x - 1)/(2^{x+1} - 3^x + 1)$, $x \in [0,1]$.

Since $h'(x) = 0$ gives

$$x = \frac{3^c - 1}{2 \cdot 2^c - 3^c + 1} k,$$

where $0 \le \frac{3^c - 1}{2 \cdot 2^c - 3^c + 1} \le 1$ (see Figure 2.1), and since $h'(0) = 2k(3^c - 1) \ge 0$ and $h'(k) = 4k(3^c - 2^c - 1) \le 0$, the function $h(x)$ has maximum x_c on $[0,k]$. Finally, since the graph of $h(x)$ is a parabola which is symmetric with respect to axis perpendicular to x, we get the result. $\square$

As shown in Figure 2.1,

$$\frac{3^x - 1}{2 \cdot 2^x - 3^x + 1} = 0$$

only if $x = 0$ (more precisely $\frac{3^x - 1}{2 \cdot 2^x - 3^x + 1} \to 0$ only if $x \to 0$) and

$$\frac{3^c - 1}{2 \cdot 2^c - 3^c + 1} = 1$$

only if $c = 1$. Hence, G_0 (G_k) maximizes σ_t^c for all $n = 4k$, $k \ge 2$, only if $c = 0$ ($c = 1$). And for every $c \in (0,1)$ there is $n_0 = 4k_0$ such that if $n = 4k$, where $k \ge k_0$, then neither G_0 nor G_k maximizes σ_t^c.

Now we turn our attention to $\sigma_t^{1/n}$, or more generally to $\sigma_t^{c/n}$. Here the situation is different.

Theorem 2.2. *Let $c \in \big[0, \frac{4}{\ln(3)}\big)$ and let $n = 4k$, where $k \geq 2$. Then a chemical graph on n vertices maximizes $\sigma_t^{c/n}$ if and only if its degree sequence is $(1^k, 2^k, 3^k, 4^k)$.*

Proof. Analogously as in the proof of Theorem 2.1, consider a real-valued function $f(x)$, such that $f(a) = \sigma_t^{c/n}(G_a)$. Then $f(x)$ achieves maximum at

$$x = \frac{3^{c/n} - 1}{2 \cdot 2^{c/n} - 3^{c/n} + 1} \cdot \frac{n}{4}.$$

Now

$$\lim_{n\to\infty} \frac{3^{c/n} - 1}{2 \cdot 2^{c/n} - 3^{c/n} + 1} \cdot \frac{n}{4} = \lim_{n\to\infty} \frac{3^{c/n} - 1}{c/n} \cdot \lim_{n\to\infty} \frac{c}{4} \cdot \lim_{n\to\infty} \frac{1}{2 \cdot 2^{c/n} - 3^{c/n} + 1} = \frac{c \cdot \ln(3)}{8},$$

and as explained in the proof of Theorem 2.1, G_0 uniquely maximizes $\sigma_t^{c/n}$ if and only if $\frac{c\cdot\ln(3)}{8} < 0.5$. $\square$

In [15], we conjectured that G_0 is the unique graph maximizing $\sigma_t^{1/n}$. Since $\frac{4}{\ln(3)} \doteq 3.640959$, Theorem 2.2 confirms this conjecture for $n \equiv 0 \pmod 4$.

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