On size of k-stepwise irregular graphs and their degree based indices

Yaser Alizadeh[a], Sandi Klavžar[b,c,d], Javaher Langari[a]

[a] Department of Mathematics, Hakim Sabzevari University, Sabzevar, Iran
y.alizadeh@hsu.ac.ir
javaher_langari61@yahoo.com

[b] Faculty of Mathematics and Physics, University of Ljubljana, Slovenia
sandi.klavzar@fmf.uni-lj.si

[c] Institute of Mathematics, Physics and Mechanics, Ljubljana, Slovenia

[d] Faculty of Natural Sciences and Mathematics, University of Maribor, Slovenia

Abstract

A graph G is k-stepwise irregular if $|d_G(u) - d_G(v)| = k$ holds for every edge uv of G. It is proved that for such a graph $m(G) \leq (n(G)^2 - k^2)/4$ holds, where the equality holds if and only if $G \cong K_{\frac{n(G)+k}{2}, \frac{n(G)-k}{2}}$. Using this result, sharp lower and upper bounds are derived for Zagreb (co)indices, the Sombor index, and the Randić index of k-stepwise irregular graphs.

Keywords: k-stepwise irregular graph; Zagreb index, Sombor index, Randić index

AMS Math. Subj. Class. (2020): 05C07, 05C09

1 Introduction

In 2018, Gutman [18] introduced *stepwise irregular graphs* as the graphs G for which the degrees of every two adjacent vertices u and v differ by one, that is, $|d_G(u)-d_G(v)| = 1$, where $d_G(w)$ is the degree of the vertex w of G, see also [2, 4, 13]. (For a related concept of stepwise transmission irregular graphs see [8, 9, 16].) Stepwise irregular graphs naturally extend to *k-stepwise irregular graphs*, $k \geq 1$, defined as the graphs G

in which $|d_G(u) - d_G(v)| = k$ holds for every edge uv. This extension was suggested for the first time in [15], where the focus was on $k = 2$. This was followed by the article [7] in which k-stepwise irregular graphs were explored for any k. One motivation behind the concept of k-stepwise irregular graphs is that this represents a new approach to analysis and understanding networks with predictable robustness or imbalance.

In the seminal paper [7] it was demonstrated that for any $k \geq 1$ and any $d \geq 2$, there exists a k-stepwise irregular graph of diameter d. Bounds for the maximum degree and for the size of k-stepwise irregular graphs were also proved. In this note we continue the investigation of k-stepwise irregular graphs by re-focusing on their maximum size and on their degree-based topological indices.

At this point, it is also necessary to mention a very similar concept, namely the *irregularity* of a graph G which was in [5] introduced as $\sum_{uv \in E(G)} |d_G(u) - d_G(v)|$ [5]. Clearly, if G is a k-stepwise irregular graph, then its irregularity is straightforward, that is, it is equal to $k \cdot |E(G)|$. Among the numerous studies dealing with graph irregularity let us point to the papers [1, 11]. The book [6] offers a broad overview of the irregularity theory of graphs.

We proceed as follows. In the next section we prove an upper bound on the size of these graphs and detect the graphs that attain the equality. In the subsequent section, we use this bound to obtain sharp lower and upper bounds for Zagreb (co)indices, the Sombor index, and the Randić index of k-stepwise irregular graphs. In the rest of the introduction we list some additional definitions needed and recall an earlier result to be applied several times later on.

Let G be a graph. Its order and size are respectively denoted by $n(G)$ and $m(G)$. When G will be clear from the context, we may simplify the notation $d_G(u)$ to $d(u)$. The number of distinct degrees in G is denoted by $C_d(G)$, and the maximum degree in G by $\Delta(G)$. We will abbreviate the term k-stepwise irregular graph to k-SI graph.

We conclude the introduction by recalling the following result which was for the special case $k = 2$ earlier proved in [15, Theorem 3].

Lemma 1.1 [7] *Every k-SI graph is bipartite.*

2 A bound on the size

In this section, we prove an upper bound on the size of k-SI graphs. We then compare this bound with the previously known bound from [7] and demonstrate that the two bonds are incomparable already within the context of the family of trees, that is, each of the two limits is better in certain cases. The new bound reads as follows.

Theorem 2.1 *If $k \geq 1$, and G is a connected k-SI graph, then*

$$m(G) \leq \frac{n(G)^2 - k^2}{4}\,,$$

where the equality holds if and only if $G \cong K_{\frac{n(G)+k}{2},\frac{n(G)-k}{2}}$.

Proof. Let $A_i = \{v:\ d_G(v) = \Delta(G) - ik\}$ and set $a_i = |A_i|$. Since G is a k-SI graph, $\{A_i:\ 0 \leq i \leq C_d(G) - 1\}$ is a partition of $V(G)$, that is,

$$\sum_{i=0}^{C_d(G)-1} a_i = n(G)\,.$$

We can therefore calculate as follows:

$$\begin{aligned} 2m(G) &= \sum_{i=0}^{C_d(G)-1} a_i(\Delta(G) - ik) \\ &= \Delta(G)\sum_{i=0}^{C_d(G)-1} a_i - ka_1 - \sum_{i=2}^{C_d(G)-1} (ika_i) \\ &\leq \Delta(G)n(G) - ka_1\,. \end{aligned}$$

A vertex from A_0 has all its neighbors in A_1, hence $a_1 \geq \Delta(G)$, and therefore,

$$m(G) \leq \frac{\Delta(G)n(G) - ka_1}{2} \leq \frac{\Delta(G)n(G) - k\Delta(G)}{2}\,, \tag{1}$$

with equality holds if and only if $C_d(G) = 2$ and $a_1 = \Delta(G)$. Consider now an edge vw, where $v \in A_0$ and $w \in A_1$. Then by Lemma 1.1, $d_G(v) + d_G(w) \leq n(G)$ and $d_G(v) - d_G(w) = k$. Since $d_G(v) = \Delta(G)$, summing these two (in)equalities we get $2\Delta(G) - k \leq n(G)$, that is, $\Delta(G) \leq (n(G) + k)/2$. Using this in (1) we obtain

$$m(G) \leq \frac{\Delta(G)(n(G) - k)}{2} \leq \frac{(n(G) + k)(n(G) - k)}{4}\,,$$

where equality holds if and only if $a_1 = \Delta(G) = \frac{n(G)+k}{2}$ and $C_d(G) = 2$. Consequently $a_0 = n(G) - a_1 = \frac{n(G)-k}{2}$. We can conclude that the equality holds if and only if $G \cong K_{\frac{n(G)+k}{2}, \frac{n(G)-k}{2}}$. □

We now compare the bound of Theorem 2.1 with [7, Theorem 5.1] which asserts that if $k \geq 1$, and G is a connected k-SI graph, then

$$m(G) \leq \frac{n(G)^2 - k^2}{4}\,, \tag{2}$$

where the equality holds if and only if $G \cong K_{\frac{n(G)+k}{2}, \frac{n(G)-k}{2}}$.

We next compare (2) with the bound of Theorem 2.1 on the class of trees. Hence let T be an arbitrary k-SI tree with. Then it follows that $\Delta(T) = (C_d - 1)k + 1$. In the special case where $C_d(T) = 2$, we obtain $T \cong K_{1,k+1}$, and in this situation both bounds coincide. Assume now that $k < n(T) - 1$, set $m = m(T)$, $\Delta = \Delta(T)$, and consider the following two functions defined for positive integers $n = n(T)$ and k:

$$\begin{aligned} f(n,k) &= \frac{n^2 - k^2}{4}, \\ g(n,k) &= \frac{n\,\Delta\,(\Delta - k)}{2\Delta - k}, \qquad \Delta = mk + 1,\ m \in \mathbb{N}. \end{aligned}$$

The equality between f and g occurs precisely when $n = 2\Delta - k$. Since $\Delta = mk + 1$, for some $m \in \mathbb{N}$, this equality point can be expressed as $n_{\text{eq}} = (2m-1)k + 2$.

To compare the size of the two functions, we observe the following cases:

- For $n < 2\Delta - k$, the quadratic growth of g dominates, so $f(n,k) < g(n,k)$.
- For $n = 2\Delta - k$, the two functions coincide, therefore $f(n,k) = g(n,k)$.
- For $n > 2\Delta - k$, the quadratic growth of f dominates, so $f(n,k) > g(n,k)$.

3 Bounds on Zagreb (co)indices

Zagreb indices represent one of the most fundamental classes of topological descriptors in mathematical chemistry, with their properties being extensively investigated since the introduction of the first Zagreb index M_1 in 1972 [21]. M_1 and its variant, the second Zagreb index M_2, are defined for a given graph G as

$$M_1(G) = \sum_{uv\in E(G)} \big(d(u)+d(v)\big)\,,$$
$$M_2(G) = \sum_{uv\in E(G)} d(u)d(v)\,.$$

A huge number of lower and upper bounds for M_1 and M_2 have been proved, the survey [12] which focuses just on lower and upper bounds for M_1 and M_2 contains more than 80 pages and lists 118 references. In this section we add to this list bounds on M_1 and M_2 for k-SI graphs, as well as bounds on the corresponding Zagreb coincides [17] which are defined by:

$$\overline{M}_1(G) = \sum_{uv\notin E(G)} \big(d(u)+d(v)\big)\,,$$
$$\overline{M}_2(G) = \sum_{uv\notin E(G)} d(u)d(v)\,.$$

Theorem 3.1 *If $k \geq 1$ and G is a connected k-SI graph, then*

$$(k+2)(n(G)-1) \leq M_1(G) \leq n(G)\frac{n(G)^2-k^2}{4}$$

and

$$(k+1)(n(G)-1) \leq M_2(G) \leq \left(\frac{n(G)^2-k^2}{4}\right)^2\,.$$

Moreover, in both cases the left equality holds if and only if $G \cong K_{1,k+1}$ and the right equality holds if and only if $G \cong K_{\frac{n(G)+k}{2},\frac{n(G)-k}{2}}$.

Proof. We first consider M_1. Since $d(u)+d(v) \geq k+2$ for each edge uv, we have:

$$M_1(G) = \sum_{uv\in E(G)} \big(d(u)+d(v)\big) \geq (k+2)m(G)\,.$$

Since G is connected, $m(G) \geq n(G)-1$, hence the left inequality. Further, the equality holds if and only if G is a k-SI tree and for each edge uv we have $|d(u)-d(v)| = k$ and

$d(u) + d(v) = k + 2$. Therefore, $d(u) = k + 1$ and $d(v) = 1$ (or the other way around), which in turn implies $G \cong K_{1,k+1}$.

Let uv be an edge of G and assume without loss of generality that $d(u) - d(v) = k$. Lemma 1.1 implies $d(u) + d(v) \leq n(G)$. From here, we get $d(u) \leq \frac{n(G)+k}{2}$ and $d(v) \leq \frac{n(G)-k}{2}$ and therefore,

$$M_1(G) = \sum_{uv \in E(G)} \big(d(u) + d(v)\big) \leq n(G)m(G)\,.$$

Then, by Theorem 2.1, $M_1(G) \leq n(G)\frac{(n(G)^2-k^2)}{4}$, where the equality holds if and only if $G \cong K_{\frac{n(G)+k}{2},\frac{n(G)-k}{2}}$. This proves the theorem for M_1.

Consider now M_2 and let uv be an edge of G with $d(u) > d(v)$. Then as in (i) we have $d(u) + d(v) \leq n(G)$ and $d(u) - d(v) = k$. The latter equality yields

$$d(u)d(v) = d(u)(d(u) - k)\,.$$

Since the function $f(x) = x^2 - kx$ is an increasing function on $x \geq k/2$, by considering $k + 1 \leq d(u) \leq \frac{n(G)+k}{2}$ we get

$$(k+1)(k+1-k)m(G) \leq M_2(G) \leq \left(\frac{n(G)+k}{2}\right)\left(\frac{n(G)+k}{2} - k\right)m(G)\,.$$

Therefore, by Theorem 2.1,

$$(k+1)(n(G)-1) \leq M_2(G) \leq \left(\frac{(n(G)^2-k^2)}{4}\right)^2\,.$$

By similar arguments as for M_1 we finally infer that the left equality holds if and only if $G \cong K_{1,k+1}$ and the right equality holds if and only if $G \cong K_{1,k+1}$. □

To derive bounds for the two Zagreb coindices, we recall the following result.

Theorem 3.2 [20] *If G is a graph, then*

$$\overline{M}_1(G) = 2m(G)(n(G)-1) - M_1(G)$$

and

$$\overline{M}_2(G) = 2m^2(G) - \frac{1}{2}M_1(G) - M_2(G)\,.$$

The bounds for the Zagreb coindices of k-SI graphs now read as follows.

Theorem 3.3 *If $k \geq 1$ and G is a k-SI graph, with $n = n(G)$ and $m = m(G)$, then*

$$(n-2)(n-1) \leq \overline{M}_1(G) \leq (2n-k-4)\left(\frac{n^2-k^2}{4}\right)$$

and

$$2m^2 - \frac{m}{4}\left(2n+n^2-k^2\right) \leq \overline{M}_2(G) \leq 2m^2 - (n-1)\left(\frac{3}{2}k+2\right).$$

Moreover, for $\overline{M}_1$, both equalities hold if and only if $G \cong K_{1,k+1}$, while the left equality for $\overline{M}_2$ holds if and only if $G \cong K_{\frac{n+k}{2},\frac{n-k}{2}}$, and the right equality for $\overline{M}_2$ holds if and only if $G \cong K_{1,k+1}$.

Proof. Consider first $\overline{M}_1$. Since for each edge uv we have $d(u)+d(v) \leq n(G)$, we get $M_1(G) \leq n(G)m(G)$. Then by the first equality of Theorem 3.2,

$$\begin{aligned}\overline{M}_1(G) &= 2(n(G)-1)m(G) - M_1(G)\\ &\geq 2(n(G)-1)m(G) - n(G)m(G) = (n(G)-2)m(G).\end{aligned}$$

G, being connected, satisfies $m(G) \geq n(G)-1$, hence

$$\overline{M}_1(G) \geq (n(G)-2)(n(G)-1).$$

Equality holds if and only if G is a star graph, which is the case when $m(G) = n(G)-1$ and $M_1(G) = n(G)m(G)$.

For the upper bound, using the bound $M_1(G) \geq (k+2)m(G)$ of Theorem 3.1, we get

$$\overline{M}_1(G) \leq 2(n(G)-1)m(G) - (k+2)m(G) = m(G)(2n(G)-k-4).$$

Hence the right inequality holds by the upper bound in Theorem 2.1. Equality holds if and only if G is both a tree and a complete bipartite graph, which occurs precisely when $G \cong K_{1,k+1}$.

Consider second $\overline{M}_2$. Applying Lemma 1.1 again to an arbitrary edge uv we have

$$d(u)+d(v) \leq n(G) \quad \text{and} \quad d(u)d(v) \leq \frac{n(G)^2-k^2}{4}. \tag{3}$$

This implies $M_1(G) \leq n(G)m(G)$ and $M_2(G) \leq \frac{n(G)^2-k^2}{4}m(G)$. Applying the second identity of Theorem 3.2, we get

$$\begin{aligned}\overline{M}_2(G) &\geq 2m^2(G) - \frac{1}{2}n(G)m(G) - \frac{n(G)^2-k^2}{4}m(G) \\ &= 2m^2(G) - m(G)\frac{n(G)^2+2n(G)-k^2}{4}\,.\end{aligned}$$

The equality holds if and only if both equalities in (3) hold for each edge, which is if and only if G is the complete bipartite graph $K_{\frac{n(G)+k}{2},\frac{n(G)-k}{2}}$.

By Theorem 3.1,

$$M_1(G) \geq (k+2)(n(G)-1) \quad \text{and} \quad M_2(G) \geq (k+1)(n(G)-1)\,.$$

Hence the right inequality is obtained by applying the second identity of Theorem 3.2:

$$\overline{M}_2(G) \leq 2m(G)^2 - \frac{1}{2}(n(G)-1)(k+2) - (n(G)-1)(k+1)\,,$$

and the equality holds if and only if $G \cong K_{1,k+1}$. □

4 Bounds on the Sombor and the Randić index

The Sombor index of a graph G, introduced by Gutman in 2021 in [19], is defined as

$$SO(G) = \sum_{uv\in E(G)} \sqrt{d(u)^2+d(v)^2}\,.$$

This graph invariant immediately received considerable attention, only a year after the seminal paper the survey paper [22] on it was published. The extraordinary interest in the Sombor index continues unabated, see, for example [3, 14, 24]. To this development we add the following result.

Theorem 4.1 *If $k \geq 1$ and G is a k-SI graph, then*

$$(k+1)\sqrt{(k+1)^2+1} \leq SO(G) \leq \left(\frac{n(G)^2-k^2}{4}\right)\sqrt{\frac{n(G)^2+k^2}{2}}\,.$$

Moreover, the left equality holds if and only if $G \cong K_{1,k+1}$ and the right equality holds if and only if $G \cong K_{\frac{n+k}{2},\frac{n-k}{2}}$.

Proof. Let uv be an edge of G where $d(u) - d(v) = k$. Thus

$$d(u)^2 + d(v)^2 = 2d(u)^2 - 2kd(u) + k^2 \,.$$

The function $f(x) = 2x^2 + k^2 - 2kx$ is an increasing function for $x \geq \frac{k}{2}$. Since $k+1 \leq d(u) \leq \frac{n(G)+k}{2}$, we derive the bounds:

$$m(G)\sqrt{(k+1)^2+1} \leq SO(G) \leq m(G)\sqrt{\left(\frac{n(G)+k}{2}\right)^2 + \left(\frac{n(G)-k}{2}\right)^2}\,.$$

Applying Theorem 2.1, the upper bound follows, while the lower bound follows since $m(G) \geq n(G) - 1 \geq (k+2) - 1 = k+1$. Moreover, the left equality holds if and only if $m(G) = n(G) - 1 = k+1$ and for each edge one endvertex is of degree $k+1$. This implies $G \cong K_{1,k+1}$. A similar argument applies to the sharpness of the upper bound. □

The Randić index [23] is one of the oldest and most widely applicable topological indices, it is defined as follows:

$$R(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u)d(v)}}\,.$$

Also this index is still the subject of considerable interest; see, for example, articles [10, 25, 26] and the references therein. Our contribution is the following result.

Theorem 4.2 *If $k \geq 1$ and G is a k-SI graph, then*

$$\frac{2(k+1)}{\sqrt{n(G)^2 - k^2}} \leq R(G) \leq \frac{n(G)^2 - k^2}{4\sqrt{k+1}}\,.$$

Moreover, both equalities hold if and only if $G \cong K_{1,k+1}$.

Proof. Let uv be an edge of G, and assume without loss of generality that $d(u) - d(v) = k$. Using analogous arguments as in the second part of the proof of Theorem 3.1, that is, to prove the bounds on $M_2(G)$, we obtain

$$k+1 \leq d(u)d(v) \leq \frac{n(G)+k}{2} \cdot \frac{n(G)-k}{2}$$

This implies

$$m(G)\frac{1}{\sqrt{\frac{n(G)^2-k^2}{4}}} \leq R(G) \leq m(G)\frac{1}{\sqrt{k+1}}\,.$$

Since $m(G) \geq k+1$, the lower bound follows, while the upper bound follows by the reuse of Theorem 2.1. We also notice that both the lower and the upper bound are sharp and the equalities hold when $G \cong K_{1,k+1}$. □

Acknowledgements

Sandi Klavžar acknowledges the financial support from the Slovenian Research and Innovation Agency ARIS (research core funding P1-0297 and projects N1-0285, N1-0355).

Declaration of interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Our manuscript has no associated data.

References

[1] H. Abdo, D. Dimitrov, I. Gutman, Graph irregularity and its measures, *Appl. Math. Comput.* **357** (2019) 317–324.

[2] D. Adiyanyam, E. Azjargal, L. Buyantogtokh, Bond incident degree indices of stepwise irregular graphs *AIMS Math.* **7** (2022) 8685–8700.

[3] S. Ahmad, K.Ch. Das, A complete solution for maximizing the general Sombor index of chemical trees with given number of pendant vertices, *Appl. Math. Comput.* **505** (2025) 129532.

[4] N. Akhter, A.Al-Hossain Ahmad, Stepwise irregular graphs and their metric-based resolvability parameters, *Math. Prob. Eng.* (2022) 3752298.

[5] M.O. Albertson, The irregularity of a graph, *Ars Combin.* **46** (1997) 219–225.

[6] A. Ali, G. Chartrand, P. Zhang, *Irregularity in Graphs*, Springer, Cham, 2021.

[7] Y. Alizadeh, S. Klavžar, J. Langari, Extremal results on k-stepwise irregular graphs, *Appl. Math. Comput.* **514** (2026) 129818.

[8] Y. Alizadeh, S. Klavžar, Z. Molaee, Generalized stepwise transmission irregular graphs, *Filomat* **38** (2024) 5875–5883.

[9] S. Al-Yakoob, D. Stevanović, On stepwise transmission irregular graphs, *Appl. Math. Comput.* **413** (2022) 126607.

[10] G. Arizmendi, D. Huerta, Energy of a graph and Randić index of subgraphs, *Discrete Appl. Math.* **372** (2025) 136–142.

[11] A. Bickle, Z. Che, Irregularities of maximal k-degenerate graphs, *Discrete Appl. Math.* **331** (2023) 70–87.

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

[13] L. Buyantogtokh, E. Azjargal, B. Horoldagva, Sh. Dorjsembe, D. Adiyanyam, On the maximum size of stepwise irregular graphs, *Appl. Math. Comput.* **392** (2021) 125683.

[14] S. Chanda, R.R. Iyer, On the Sombor index of Sierpiński and Mycielskian graphs, *Commun. Comb. Optim.* **10** (2025) 20–56.

[15] S. Das, U. Mishra, S. Rai, On two-stepwise irregular graphs, *Sci. Iran.* **30** (2023) 1049–1057.

[16] A.A. Dobrynin, R. Sharafdini, Stepwise transmission irregular graphs, *Appl. Math. Comput.* **371** (2020) 124949.

[17] T. Doslić, Vertex-weighted Wiener polynomials for composite graphs, *Ars Math. Contemp.* **1** (2008) 66–80.

[18] I. Gutman, Stepwise irregular graphs, *Appl. Math. Comput.* **325** (2018) 234–238.

[19] I. Gutman, Geometric approach to degree–based topological indices: Sombor indices, *MATCH Commun. Math. Comput. Chem.* **86** (2021) 11–16.

[20] I. Gutman, B. Furtula, Z.K. Vukićević, G. Popivoda, On Zagreb indices and coindices, *MATCH Commun. Math. Comput. Chem.* **74** (2015) 5–16.

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

[22] H. Liu, I. Gutman, L. You, Y. Huang, Sombor index: review of extremal results and bounds, *J. Math. Chem.* **60** (2022) 771–798.

[23] M. Randić, Characterization of molecular branching, *J. Amer. Chem. Soc.* **97** (1975) 6609–6615.

[24] S. Rabizadeh, M. Habibi, I. Gutman, Some notes on Sombor index of graphs, *MATCH Commun. Math. Comput. Chem.* **93** (2025) 853–859.

[25] E. Swartz, T. Vetrík, General sum-connectivity index and general Randić index of trees with given maximum degree, *Discrete Math. Lett.* **12** (2023) 181–188.

[26] M. Yuan, Limiting distribution for the Randić index of a random geometric graph, *MATCH Commun. Math. Comput. Chem.* **93** (2025) 767–789.