MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **76** (2016) 81-98

ISSN 0340 - 6253

Maximum Size of Maximally Irregular Graphs

Batmend Horoldagva[1,2,*], **Lkhagva Buyantogtokh**[2], **Shiikhar Dorjsembe**[1], **Ivan Gutman**[3,4]

[1]*Department of Mathematics, National University of Education, Baga toiruu-14, Ulaanbaatar, Mongolia*
horoldagva@msue.edu.mn , shiihardorjsembe@yahoo.com

[2]*Department of Mathematics, Sungkyunkwan University, Suwon 440-746, Republic of Korea*
buyantogtokh.lhag@yahoo.com

[3]*Faculty of Science, University of Kragujevac, Kragujevac, Serbia*
gutman@kg.ac.rs

[4]*State University of Novi Pazar, Novi Pazar, Serbia*

(Received February 8, 2016)

Abstract

The irregularity index of a simple graph G is the number of distinct elements in the degree sequence of G. If the irregularity index of a connected graph G is equal to the maximum vertex degree, then G is said to be maximally irregular. In this paper, we determine the maximum size of maximally irregular graphs with given order and irregularity index.

1 Introduction

Let $G = (V, E)$ be a connected simple graph with vertex set $V = V(G)$ and edge set $E = E(G)$. Let G has $n = |V(G)|$ vertices and $m = |E(G)|$ edges. The degree $d_G(v)$ of a vertex v of G is the number of vertices adjacent to v. The degree sequence of

*Corresponding author

a graph is the non-increasing sequence of the degrees of the vertices. The maximum degree Δ of a graph G is the maximum value of the degrees of vertices.

A graph G is is said to be regular if all its vertices have the same degree. Regular graphs played an outstanding role in the history of graph theory [11] and are still in the focus of interest of mathematicians. In mathematical chemistry, the importance of regular graphs has much increased after the discovery of fullerenes and nanotubes. A graph that is not regular is said to be irregular. In numerous applications of graph theory, it is necessary to know how irregular a given graph is, or – what is the same – there is a need for a (numerical) measure of irregularity.

In 1988, Chartrand, Erdős and Oellermann [12] posed a question "*Which class of graphs is opposite to the regular graphs?*" According to them, a simple connected graph is highly irregular if each of its vertices is adjacent only to vertices with distinct degrees. The class of highly irregular graphs was studied in [6, 25, 26]. Majcher and Michael [26] mention that during the Second Kraków Conference on Graph Theory (1994), Erdős asked a question about extreme sizes of highly irregular graphs of given order. The degree sequence of highly irregular graphs was studied in [25].

Any measure of graph irregularity, say $\mathcal{I}(G)$, must satisfy the following requirements:

(i) $\mathcal{I}(G) = 0$ if and only if the (connected) graph G is regular.
(ii) $\mathcal{I}(G) > 0$ if the (connected) graph G is not regular.
(iii) The quantity $\mathcal{I}$ is defined so that its numerical value follows our intuitive feeling for "deviating from being regular".

It may be that the first such measure of graph irregularity is found in the seminal paper of Collatz and Sinogowits [14].

Let λ_1 be the greatest eigenvalue of the adjacency matrix. Then the Collatz–Sinogowitz irregularity measure is

$$CS(G) = \lambda_i - \frac{2m}{n}\,.$$

Another direction of approaching the irregularity is via the *imbalance* (or irregularity) of edges. The imbalance of an edge $e = uv \in E$ is defined as $|d_G(u) - d_G(v)|$ [8,13].

In [7], Albertson defined the irregularity of a graph G as

$$irr(G) = \sum_{uv \in E(G)} |d_G(u) - d_G(v)|$$

which is usually referred to as the *Albertson index*, although Fath–Tabar re-named it third Zagreb index [19]. A similar, yet not much studied quantity would be [20]

$$irr_2(G) = \sum_{uv \in E(G)} \left[d_G(u) - d_G(v)\right]^2 .$$

Recently [1,3] the *total irregularity* was introduced, defined as

$$irr_t(G) = \sum_{\{u,v\} \subseteq V(G)} |d_G(u) - d_G(v)| .$$

Bell [10] measured the irregularity of a graph by means of the variance of its vertex degrees. Thus, his irregularity measure is

$$Var(G) = \frac{1}{n} \sum_{v \in V(G)} \left(d_i - \frac{2m}{n}\right)^2$$

recalling that the average value of vertex degrees is $2m/n$.

The above irregularity measures are also related to the two Zagreb indices $M_1(G)$ and $M_2(G)$, and the F-index [17,20,22]

$$\begin{aligned} M_1(G) &= \sum_{v \in V(G)} d_G(v)^2 \\ M_2(G) &= \sum_{uv \in E(G)} d_G(u)\, d_G(v) \\ F(G) &= \sum_{v \in V(G)} d_G(v)^3 . \end{aligned}$$

Namely,

$$Var(G) = \frac{1}{n} M_1(G) - \left(\frac{2m}{n}\right)^2$$

and

$$irr_2(G) = F(G) - 2M_2(G) .$$

For comparative studies of CS, irr, irr_t, and Var see [10, 15, 16, 21]. For more information on the above specified irregularity measures see the recent papers [1–4, 16, 17, 20, 22] and the references cited therein.

2 Irregularity index

A simple, straightforward, and completely different way of expressing the irregularity of graphs is via their *irregularity index*, equal to the the number of distinct elements in the degree sequence. This concept was, in an implicit manner, used in the early works [5,6,25,26], but was explicitly considered only quite recently [24,27,28]. In the present paper we offer a few new results on this index.

Graphs whose all vertices have different degrees were referred to as *perfect*. For such graphs, the irregularity index would be equal to the number of vertices. A classical result of Behzad and Chartrand [9] establishes that there are no perfect graphs.

Clearly, for any connected graph G, the irregularity index of G is less than or equal to the maximum degree. If the irregularity index of a connected graph G is equal to the maximum degree, then G is said to be *maximally irregular*.

Mukwembi [28] proved that every highly irregular graph is maximally irregular and established an asymptotically tight upper bound on the size of maximally irregular graphs of given order. Also, he studied a class of maximally irregular triangle–free graphs and conjectured that if G is a maximally irregular triangle–free graph of order n, then $|E(G)| \leq n(n+1)/6$. Recently, Liu et al. [24] proved this conjecture and gave a tight upper bound on the size of maximally irregular graphs.

For given integers n and t such that $1 < t < n$, we denote by $\mathcal{M}_{n,t}$ the class of all maximally irregular graphs of order n with irregularity index t. For a given positive integer n, we denote

$$\xi(n) = n - \frac{1}{2}\left(\sqrt{4n+3-2(-1)^n} - 1\right). \tag{1}$$

In this paper, first, we show that $\mathcal{M}_{n,t} \neq \emptyset$ for all integers n and t such that $1 < t < n$. In addition, for $t \geq \xi(n)$, we prove that the maximum size of a graph in $\mathcal{M}_{n,t}$ is equal to $\lfloor \frac{n^2}{4} \rfloor$. Further for $t \leq \xi(n)$, we characterize the degree sequence of maximally irregular graphs in $\mathcal{M}_{n,t}$ that achieve maximum size. Moreover, we give a tight upper bound on the size of maximally irregular graphs in terms of order and irregularity index.

3 Existence of maximally irregular graphs in $\mathcal{M}_{n,t}$ and the maximum size when $t \geq \xi(n)$

As already mentioned, there exist no graphs with all degrees different. A degree sequence is quasi–perfect if exactly two of its elements are same. The respective graphs are also referred to as quasi–perfect. Behzad and Chartrand [9] showed that there are exactly two quasi–perfect graphs of order n for each $n > 1$ and these two graphs are mutually complementary.

Theorem 1 (Behzad & Chartrand)**.** *For each $n > 1$, there is a unique connected quasi–perfect graph of order n and its degree sequence is*

$$\Big[n-1, n-2, \ldots, \lfloor n/2 \rfloor, \lfloor n/2 \rfloor, \ldots, 2, 1\Big].$$

From the above theorem, it follows that the connected quasi–perfect graph of order n is maximally irregular and its the irregularity index is $n-1$. Note that P_2 is the unique maximally irregular graph with irregularity index 1 and the irregularity index of a graph is less than its order. Thus we consider the graphs of order n with irregularity index t satisfying $1 < t < n$.

Proposition 1. *For given integers n and t such that $1 < t < n$, there exists a maximally irregular graph of order n with irregularity index t. i.e., $\mathcal{M}_{n,t} \neq \emptyset$.*

Proof. By Theorem 1, there is a connected quasi–perfect graph of order $t+1$ (say, G_{t+1}) and its degree sequence is

$$\Big[t, t-1, \ldots, \lfloor (t+1)/2 \rfloor, \lfloor (t+1)/2 \rfloor, \ldots, 2, 1\Big].$$

If $n = t+1$, then $G_{t+1} \in \mathcal{M}_{t+1,t}$, that is, $\mathcal{M}_{n,t} \neq \emptyset$.

Then, suppose that $t+1 < n$. Let G_{t+2} be a graph obtained from G_{t+1} by adding a new vertex v_{t+2} and joining it to each vertex of degree $t-1, \ldots, \lfloor (t+1)/2 \rfloor + 1, \lfloor (t+1)/2 \rfloor$ in G_{t+1} except one vertex of degree $\lfloor (t+1)/2 \rfloor$. Then $d_{G_{t+2}}(v_{t+2}) = \lfloor t/2 \rfloor$ and the degree sequence of G_{t+2} is

$$\Big[t, t, t-1, \ldots, \lfloor t/2 \rfloor, \lfloor t/2 \rfloor, \ldots, 2, 1\Big].$$

Hence $G_{t+2} \in \mathcal{M}_{t+2,\,t}$.

If $n = t+2$, then we are done. Otherwise, we add a vertex v_{t+3} and join it to each vertex of degree $t-1, \ldots, \lfloor t/2 \rfloor + 1, \lfloor t/2 \rfloor$ in G_{t+2} except one vertex of degree $\lfloor t/2 \rfloor$. Then $d_{G_{t+3}}(v_{t+3}) = \lfloor (t+1)/2 \rfloor$. Therefore, the degree sequence of G_{t+3} is

$$\Big[t, t, t, t-1, \ldots, \lfloor (t+1)/2 \rfloor, \lfloor (t+1)/2 \rfloor, \ldots, 2, 1\Big].$$

and it follows that $G_{t+3} \in \mathcal{M}_{t+3,\,t}$.

Repeating the above algorithm, we always arrive at a graph G_n of order n with degree sequence either

$$\Big[\underbrace{t, t, ..., t}_{n-t}, t-1, \ldots, \lfloor (t+1)/2 \rfloor, \lfloor (t+1)/2 \rfloor, \ldots, 2, 1\Big]$$

if $n-t$ is odd, or

$$\Big[\underbrace{t, t, ..., t}_{n-t}, t-1, \ldots, \lfloor t/2 \rfloor, \lfloor t/2 \rfloor, \ldots, 2, 1\Big]$$

if $n-t$ is even.

Clearly, G_n is connected by the construction. Thus we have $G_n \in \mathcal{M}_{n,t}$. This completes the proof. □

Let $\mathcal{M}_n$ be a class of maximally irregular graphs of order n, which was defined in [24]. Then for any graph $G \in \mathcal{M}_n$, we have the following.

(i) $V(G)$ can be partitioned into $X \cup Y$ such that $|X| = \lfloor n/2 \rfloor$ and $|Y| = \lceil n/2 \rceil$. Furthermore, the vertices in X have degrees $1, 2, \ldots, \lfloor n/2 \rfloor$.

(ii) $G[X]$ is an empty graph and $G[Y]$ is a complete graph, where $G[X]$ denotes the subgraph of G induced by X.

(iii) For any positive integer $k \leq \Delta$, there exists a vertex $v \in V(G)$ such that $d_G(v) = k$.

Mukwembi [28] proved that if G is a maximally irregular graph of order n, then $|E(G)| \leq (n-1)(n+2)/4$. Recently, Liu et al. [24] improved this bound and gave the following result.

Theorem 2 (Liu et al)**.** *Let G be a maximally irregular graph of order n. Then $|E(G)| \leq \lfloor \frac{n^2}{4} \rfloor$ with equality holding if and only if $G \in \mathcal{M}_n$.*

By the definition of $\mathcal{M}_n$ and Theorem 2, the connected quasi–perfect graph of order n belongs to $\mathcal{M}_n \setminus \mathcal{M}_{n,t}$ for all $1 < t < n-1$. The size and irregularity index of the connected quasi–perfect graph of order n are equal to $\lfloor \frac{n^2}{4} \rfloor$ and $n-1$, respectively. Therefore $\mathcal{M}_n \setminus \mathcal{M}_{n,t} \neq \emptyset$ for all $1 < t < n-1$.

Theorem 3. *Let n and t be integers such that $1 < t < n$. Then $\mathcal{M}_{n,t} \cap \mathcal{M}_n \neq \emptyset$ if and only if $t \geq \xi(n)$.*

Proof. Suppose that $\mathcal{M}_{n,t} \cap \mathcal{M}_n \neq \emptyset$. Let G be a graph in $\mathcal{M}_{n,t} \cap \mathcal{M}_n$. Then since $G \in \mathcal{M}_{n,t}$, we have $2|E(G)| \leq \sum\limits_{i=1}^{t} i + (n-t)t$. Also since $G \in \mathcal{M}_n$, we have $|E(G)| = \lfloor \frac{n^2}{4} \rfloor$. Therefore from the above, it follows that

$$\sum_{i=1}^{t} i + (n-t)t \geq 2 \left\lfloor \frac{n^2}{4} q \right\rfloor . \tag{2}$$

Thus, from (1) one can see easily that the inequality (2) is equivalent to $t \geq \xi(n)$.

Suppose that $t \geq \xi(n)$. Then we prove that there exists a graph G in $\mathcal{M}_{n,t} \cap \mathcal{M}_n$.

Consider two sets of vertices $X = \{x_1, x_2, \ldots, x_{\lfloor n/2 \rfloor}\}$ and $Y = \{y_1, y_2, \ldots, y_{\lceil n/2 \rceil}\}$. Let us construct a graph H of order n as follows:

(i) X is an independent set and Y is a clique in H,

(ii) For i such that $i \geq n-t$, x_i and y_j are adjacent if and only if $j \leq i$.

By the construction, $x_1, x_2, \ldots, x_{n-t-1}$ are isolated vertices in H and $d_H(x_i) = i$ for $n-t \leq i \leq \lfloor n/2 \rfloor$. Now, we calculate the degrees of the vertices in Y. If $i \leq n-t$ then the vertex y_i has $\lceil n/2 \rceil - 1$ neighbors in Y and $\lfloor n/2 \rfloor - (n-t-1)$ neighbors in X. Then it follows that $d_H(y_i) = t$ for all $i \leq n-t$. If $i > n-t$, then the vertex y_i has $\lceil n/2 \rceil - 1$ neighbors in Y and $\lfloor n/2 \rfloor - i + 1$ neighbors in X. Therefore, $d_H(y_i) = n-i$ for $n-t < i \leq \lceil n/2 \rceil$. From the above the degree sequence of H is

$$\Big[\underbrace{t, \ldots, t}_{n-t}, \underbrace{t-1, t-2, \ldots, \lfloor n/2 \rfloor}_{\lceil n/2 \rceil - (n-t)}, \lfloor n/2 \rfloor, \lfloor n/2 \rfloor - 1, \ldots, n-t, \underbrace{0, \ldots, 0}_{n-t-1}\Big] . \tag{3}$$

On the other hand, it is easy to see that the inequality $\xi(n) \leq t$ is equivalent to

$$\sum_{i=1}^{n-t-1} i \leq \left\lceil \frac{n}{2} \right\rceil - (n-t).$$

Hence we construct a new graph G of order n by adding $\sum_{i=1}^{n-t-1} i$ edges to H. For each i such that $i \leq n-t-1$, x_i and y_j are adjacent in G if and only if $\lceil n/2 \rceil - i(i+1)/2 < j \leq \lceil n/2 \rceil - i(i-1)/2$. Then $d_G(x_i) = i$ for $1 \leq i \leq n-t-1$ and $d_G(y_j) = d_H(y_j)+1$ for $\lceil n/2 \rceil + 1 - \sum_{i=1}^{n-t-1} i \leq j \leq \lceil n/2 \rceil$. Thus from (3), the degree sequence of G is defined as follows

$$\Big[\underbrace{t,\ldots,t}_{n-t}, t-1, t-2, \ldots, t-q, t-q, \ldots, \lfloor n/2 \rfloor + 1, \lfloor n/2 \rfloor, \lfloor n/2 \rfloor - 1, \ldots, 2, 1\Big] \quad (4)$$

where $q = \lceil n/2 \rceil - (n-t) - \sum_{i=1}^{n-t-1} i$. Therefore, $G \in \mathcal{M}_{n,t}$. From (4), we get

$$|E(G)| = \frac{1}{2}\left(\sum_{i=1}^{t-1} i + (n-t)t + t - q\right) = \left\lfloor \frac{n^2}{4} \right\rfloor.$$

Hence $G \in \mathcal{M}_n$ by Theorem 2. This completes the proof. □

Corollary 2. *Let n and t be integers such that $1 < t < n$. If $t \geq \xi(n)$ and $n - t > 2$ then $\mathcal{M}_{n,t} \setminus \mathcal{M}_n \neq \emptyset$.*

Proof. Since $t \geq \xi(n)$, there exists a graph G in $\mathcal{M}_{n,t} \cap \mathcal{M}_n$ which realizes the sequence (4) by Theorem 3. Therefore there are vertices u and v in G such that $d_G(u) = d_G(u) = t$ because we have $n - t > 2$. By the construction of G, $uv \in E(G)$. Let G' be a graph obtained from G by deleting an edge uv. Then clearly $G' \in \mathcal{M}_{n,t}$ and $G \notin \mathcal{M}_n$. Hence the corollary. □

We now give an interesting result on the class $\mathcal{M}_{n,t}$. Namely, from this result it follows that the maximum size of a graph in $\mathcal{M}_{n,t}$ depends only on the order n when $t \geq \xi(n)$.

Theorem 4. *Let n and t be integers such that $1 < t < n$. If $t \geq \xi(n)$, then the maximum size of a graph in $\mathcal{M}_{n,t}$ is equal to $\lfloor \frac{n^2}{4} \rfloor$.*

Proof. Since $t \geq \xi(n)$, there exists a graph G in $\mathcal{M}_{n,t} \cap \mathcal{M}_n$. Since $G \in \mathcal{M}_n$, we have $|E(G)| = \lfloor \frac{n^2}{4} \rfloor$ by the definition of $\mathcal{M}_n$. By Theorem 2, $|E(H)| \leq \lfloor \frac{n^2}{4} \rfloor$ for all H in $\mathcal{M}_{n,t}$ such that $1 < t < n$. Therefore G has the maximum size in $\mathcal{M}_{n,t}$. This completes the proof. □

4 Degree sequence of maximally irregular graphs in $\mathcal{M}_{n,t}$ and the maximum size when $t \le \xi(n)$

A sequence $d = [d_1, d_2, \ldots, d_n]$ is said to be graphic if there exists a graph whose degree sequence is d. Let $d = [d_1, d_2, \ldots, d_n]$ be a non-increasing sequence of non-negative integers and k be any integer such that $1 \le k \le n$. Let d' be the sequence obtained from d by deleting d_k and by setting $d'_i = d_i - 1$ for the d_k largest elements of d other than d_k. This operation of getting d' is called laying off d_k and d' is called the residual sequence by laying off d_k; for more details see [29] and the references cited therein. There are several characterizations of a graphic sequence and we apply two of them to characterize the degree sequence of maximally irregular graphs for which gives the maximum size. Havel and Hakimi independently obtained recursive necessary and sufficient conditions for a degree sequence, in terms of laying off a largest integer in the sequence. Kleitman and Wang [23] proved the necessary and sufficient conditions for arbitrary layoffs.

Theorem 5 (Kleitman & Wang)**.** *A non-increasing sequence of non-negative integers is graphic if and only if the residual sequence obtained by laying off any non-zero element of the sequence is graphic.*

The following result is the well known combinatorial characterization of graphic sequences, due to Erdős and Gallai [18].

Theorem 6 (Erdős & Gallai)**.** *Let $d = [d_1, d_2, \ldots, d_n]$ be a non-increasing sequence of non-negative integers. Then the sequence d is graphic if and only if $\sum_{i=1}^{n} d_i$ is even and the inequalities*

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

hold for each k such that $1 \le k \le n$.

Let n and t be integers such that $1 < t < n$. If $t \ge \xi(n)$, then the constructed graph G in Theorem 3 has maximum size in $\mathcal{M}_{n,t}$ and its degree sequence is defined by (4). We now characterize the degree sequence of graphs in the class $\mathcal{M}_{n,t}$ such that $t \le \xi(n)$ that achieve the maximum size. Note that the size of a graph is maximum if and only if the sum of elements of its degree sequence is maximum. Let $t \leq \xi(n)$ then we consider the following two sequences

$$\Big[\underbrace{t, t, \ldots, t}_{n-t+1}, t-1, \ldots, 2, 1\Big] \tag{5}$$

and

$$\Big[\underbrace{t, t, \ldots, t}_{n-t}, t-1, t-1, \ldots, 2, 1\Big] \tag{6}$$

where $1 < t < n$. If the sequence (5) is graphic, then obviously it achieves maximum size in $\mathcal{M}_{n,t}$. Thus, we now study the above two sequences.

Lemma 3. *Let n and t be integers such that $1 < t < n$. If $t \leq \xi(n)$, then $\sum_{i=1}^{n-t} i \geq \lceil n/2 \rceil$ with equality holding if and only if $t = \xi(n)$.*

Proof. Since $t \leq \xi(n)$, we have $n - t \geq n - \xi(n)$. Thus $\sum_{i=1}^{n-t} i = (n-t)(n-t+1)/2 \geq (n - \xi(n))(n - \xi(n) + 1)/2 = \lceil n/2 \rceil$ by using (1) and it is easy to see that the equality holds if and only if $t = \xi(n)$. □

The following result is useful for our main results in this section.

Proposition 4. *Let n and t be integers such that $1 < t < n$. If $\lfloor n/2 \rfloor \leq t \leq \xi(n)$, then*

(i) the sequence

$$\Big[\underbrace{\lceil n/2 \rceil, \lceil n/2 \rceil, \ldots, \lceil n/2 \rceil}_{\lceil n/2 \rceil}, n-t, \ldots, 2, 1\Big] \tag{7}$$

is graphic if and only if the sum of the elements of (7) is even.

(ii) the sequence

$$\Big[\underbrace{\lceil n/2 \rceil, \lceil n/2 \rceil, \ldots, \lceil n/2 \rceil}_{\lceil n/2 \rceil}, n-t+1, n-t-1, \ldots, 2, 1\Big] \tag{8}$$

is graphic if and only if the sum of the elements of (8) is even.

Proof. Since (7) and (8) are graphic, the sums of their elements are even. Conversely, suppose that the sums of the elements of (7) and (8) are even.

(i) By using the Erdős–Gallai theorem, we show that (7) is graphic. Since $\lfloor n/2 \rfloor \leq t < n$, (7) is the non-increasing sequence of positive integers. For convenience we denote the sequence (7) by $d_1, d_2, \ldots, d_s$, where $d_1 \geq d_2 \geq \cdots \geq d_s$ and $s = \lceil n/2 \rceil + n - t$. Then

$$d_i = \left\lceil \frac{n}{2} \right\rceil \text{ for } 1 \leq i \leq \left\lceil \frac{n}{2} \right\rceil \quad \text{and} \quad d_i = s - i + 1 \;\text{ for }\; \left\lceil \frac{n}{2} \right\rceil < i \leq s. \tag{9}$$

Case 1. Let $k > \lceil n/2 \rceil$. Then by (9), $k - 1 \geq \lceil n/2 \rceil$ and $d_i \leq \lceil n/2 \rceil$ for $1 \leq i \leq s$. Therefore,

$$k(k-1) + \sum_{i=k+1}^{s} \min(k, d_i) \geq k(k-1) \geq k \left\lceil \frac{n}{2} \right\rceil \geq \sum_{i=1}^{k} d_i\,.$$

Case 2. Let $k \leq \lceil n/2 \rceil$. Then by (9), $\min(k, d_i) = k$ for $k \leq i \leq \lceil n/2 \rceil$. Therefore,

$$\begin{aligned} k(k-1) + \sum_{i=k+1}^{s} \min(k, d_i) &= k(k-1) + k\left(\left\lceil \frac{n}{2} \right\rceil - k\right) + \sum_{i=\lceil n/2 \rceil + 1}^{s} \min(k, d_i) \\ &= k\left\lceil \frac{n}{2} \right\rceil - k + \sum_{i=\lceil n/2 \rceil + 1}^{s} \min(k, d_i) \\ &= \sum_{i=1}^{k} d_i - k + \sum_{i=\lceil n/2 \rceil + 1}^{s} \min(k, d_i) \end{aligned} \tag{10}$$

since $d_i = \lceil n/2 \rceil$ for $1 \leq i \leq \lceil n/2 \rceil$ and $k \leq \lceil n/2 \rceil$. Hence, it is sufficient to prove that

$$\sum_{i=\lceil n/2 \rceil + 1}^{s} \min(k, d_i) - k \geq 0\,. \tag{11}$$

If $k < n - t$, then (11) holds because $d_{\lceil n/2 \rceil + 1} = n - t$ and $\min(k, d_{\lceil n/2 \rceil + 1}) = k$. If $k \geq n - t$, then $\min(k, d_i) = d_i$ for $\lceil n/2 \rceil + 1 \leq i \leq s$. Therefore from $t \leq \xi(n)$ and $k \leq \lceil n/2 \rceil$ we get

$$\sum_{i=\lceil n/2 \rceil + 1}^{s} \min(k, d_i) = \sum_{i=\lceil n/2 \rceil + 1}^{s} d_i = \sum_{i=1}^{n-t} i \geq \left\lceil \frac{n}{2} \right\rceil \geq k \tag{12}$$

by using (9) and Lemma 3. Thus, in this case, the Erdős–Gallai inequalities hold from (10). Hence, it follows that (7) is graphic.

(*ii*) Let n be odd. Then, consider the following sequence

$$\Big[\underbrace{\lceil (n-1)/2 \rceil, \lceil (n-1)/2 \rceil, \ldots, \lceil (n-1)/2 \rceil}_{\lceil (n-1)/2 \rceil}, n - t, \ldots, 2, 1\Big]\,. \tag{13}$$

It is easy to see that the difference of the sum of the elements in (8) and (13) equals to $2\lceil n/2\rceil$. Hence the sum of the elements of (13) is even. On the other hand, from the hypothesis of this Proposition we have $\lfloor (n-1)/2\rfloor \le t-1 \le \xi(n)-1 \le \xi(n-1)$. Therefore, the sequence (13) is graphic by Proposition 4 (i) and it is the residual sequence by laying off a element $\lceil n/2\rceil$ of the sequence (8). Thus the sequence (8) is graphic by the Kleitman–Wang theorem.

Let now n be even. Then we consider the sequence

$$\Big[\underbrace{\lceil (n-2)/2\rceil, \lceil (n-2)/2\rceil, \ldots, \lceil (n-2)/2\rceil}_{\lceil (n-2)/2\rceil}, n-t, \ldots, 2, 1\Big] \tag{14}$$

and proceeding similarly as above, prove that (8) is graphic. This completes the proof. □

Lemma 5. *Let n and t be integers such that $1 < t < n$. If $t > \xi(n)$, then (7) and (8) are not graphic.*

Proof. Since $t > \xi(n)$, by Lemma 3 we have $\sum_{i=1}^{n-t} i < \lceil n/2\rceil$. Therefore, from (10) and (12) when $k = \lceil n/2\rceil$, we get the opposite of the Erdős–Gallai inequality . Therefore, (7) and (8) are not graphic. □

A sequence d is potentially graphic if there is a connected graph with degree sequence d.

Lemma 6. *If the sequences* (5) *and* (6) *are graphic, then they are potentially graphic.*

Proof. We follow an argument used in [29]. Since the sequence (5) is graphic, there is a graph H with degree sequence (5). Suppose that H is disconnected and let C_i and C_j be components of H. The unique vertex of H has degree 1 and degrees of others are greater than 1 because we have $1 < t < n$. Therefore, each component of H contains a cycle. Let u_iv_i be an edge of a cycle in the component C_i and u_jv_j be an edge in C_j. We now delete the edges u_iv_i and u_jv_j of H, and add the edges u_iv_j and v_iu_j. Then the obtained graph has same degree sequence as H and the number of components subtracted by 1. By repeating the above operation we arrive at a connected graph. Thus the sequence (5) is potentially graphic. Similarly, the sequence (6) is also potentially graphic. □

Since the sum of elements of the sequence (5) is even, it follows that $t(2n-t+1) \equiv 0\ (mod\ 4)$. It is easy to check that $t(2n-t+1) \equiv 0\ (mod\ 4)$ if and only if $t \equiv 0\ (mod\ 4)$, or $t \equiv 1\ (mod\ 4)$ and $n \equiv 0\ (mod\ 2)$, or $t \equiv 3\ (mod\ 4)$ and $n \equiv 1\ (mod\ 2)$. Also, since the sum of elements of the sequence (6) is even, $t(2n-t+1) \equiv 2\ (mod\ 4)$. Thus $t(2n-t+1) \equiv 2\ (mod\ 4)$ if and only if $t \equiv 2\ (mod\ 4)$, or $t \equiv 1\ (mod\ 4)$ and $n \equiv 1\ (mod\ 2)$, or $t \equiv 3\ (mod\ 4)$ and $n \equiv 0\ (mod\ 2)$. Therefore, for the given integers n and t such that $1 < t < n$, we always get a sequence either (5) or (6) in which its the sum of elements is even.

We say that a sequence d is MI-graphic if there exists a maximally irregular graph which realizes the sequence d .

Theorem 7. *Let n and t be integers such that $1 < t < n$. Then*
(i) the sequence (5) is MI-graphic if and only if $t \leq \xi(n)$ and $t(2n-t+1) \equiv 0\ (mod\ 4)$.
(ii) the sequence (6) is MI-graphic if and only if $t \leq \xi(n)$ and $t(2n-t+1) \equiv 2\ (mod\ 4)$.

Proof. ($\Leftarrow$) Let $t \leq \xi(n)$. It is easy to see that since $t(2n-t+1) \equiv 0\ (mod\ 4)$ and $t(2n-t+1) \equiv 2\ (mod\ 4)$, the sums of the elements in (5) and (6) are even. Now, we prove that (5) and (6) are MI-graphic. We distinguish the following two cases.

Case 1. $t \leq \lfloor n/2 \rfloor$.

We consider a non-increasing sequence $d = [d_1, d_2, \ldots, d_n]$ such that

$$d_{\ell+1} = t-1,\ d_n = 1 \text{ and } d_i = t \text{ for } 1 \leq i \leq \ell \text{ where } \ell = n-t+1 \text{ or } \ell = n-t\,. \quad (15)$$

Now, we prove that the sequence d satisfies the Erdős–Gallai inequalities.

Since $t \leq \lfloor n/2 \rfloor$, we have

$$\ell \geq t. \quad (16)$$

Suppose, first, that $k > \ell$. Then clearly $k-1 \geq \ell$ and $d_i \leq t$ for $1 \leq i \leq n$ from (15). Using these inequalities and (16), we get

$$k(k-1) + \sum_{i=k+1}^{n} \min(k, d_i) \geq k\ell + \sum_{i=k+1}^{n} \min(k, d_i) \geq k\ell \geq kt \geq \sum_{i=1}^{k} d_i\,.$$

Suppose, now, that $k \leq \ell$.

If $k < t$, then we have $\min(k, d_i) = k$ for $k < i \leq \ell + 1$ and $d_i = t$ for $1 \leq i \leq \ell$ from (15). Therefore,

$$\begin{aligned} k(k-1) + \sum_{i=k+1}^{n} \min(k, d_i) &= k(k-1) + k(\ell+1-k) + \sum_{i=\ell+2}^{n} \min(k, d_i) \\ &= k\ell + \sum_{i=\ell+2}^{n} \min(k, d_i) > k\ell \geq kt = \sum_{i=1}^{k} d_i \end{aligned}$$

from (16) and $k \leq \ell$.

If $k = t$, then $\min(k, d_{\ell+1}) = t - 1$ and $\min(k, d_n) = 1$ from (15). Therefore,

$$k(k-1) + \sum_{i=k+1}^{n} \min(k, d_i) \geq k(t-1) + t = kt = \sum_{i=1}^{k} d_i$$

from (16) and $k \leq \ell$.

If $k > t$, then we have $k - 1 \geq t$, $\min(k, d_i) = d_i$ and $d_i \leq t$ for $1 \leq i \leq n$ from (15). Therefore,

$$k(k-1) + \sum_{i=k+1}^{n} \min(k, d_i) = k(k-1) + \sum_{i=k+1}^{n} d_i \geq k(k-1) \geq kt = \sum_{i=1}^{k} d_i$$

since $k < \ell$.

From the above, the sequence d satisfies the Erdős–Gallai inequalities. Hence (5) and (6) also satisfy the Erdős–Gallai inequalities. Therefore since the sums of the elements in (5) and (6) are even, (5) and (6) are graphic.

Case 2. $\lfloor n/2 \rfloor < t \leq \xi(n)$.

(i) Since $t > \lfloor n/2 \rfloor$, there exists an element $n - t + 1$ in (5) which is equal to the number of t. Then by laying off the element $n - t + 1$ of the sequence (5), we get the residual sequence

$$\Big[\underbrace{t-1, t-1, \ldots, t-1}_{n-t+2}, t-2, \ldots, n-t+2, n-t, n-t-1, \ldots, 2, 1\Big].$$

Again by laying off the element $n - t + 2$ of the above sequence, we get

$$\Big[\underbrace{t-2, t-2, \ldots, t-2}_{n-t+3}, t-3, \ldots, n-t+3, n-t, n-t-1, \ldots, 2, 1\Big].$$

Repeating the above described algorithm, we arrive at the sequence (7). By Proposition 4 (i), the sequence (7) is graphic. Thus (5) is graphic by the Kleitman–Wang theorem.

(ii) Similarly, by using the laying off operation to the sequence (6) we get the sequence (8). By Proposition 4 (ii), the sequence (8) is graphic. Thus the sequence (6) is graphic from the Kleitman–Wang theorem.

Since (5) and (6) are graphic, by Lemma 6 they are potentially graphic. Therefore, the sequences (5) and (6) are MI-graphic.

($\Rightarrow$) Let (5) and (6) be MI-graphic. Suppose that $t > \xi(n)$. Then by Lemma 5, (7) and (8) are not graphic. Therefore it follows that from *Case* 2, (5) and (6) are not graphic by the Kleitman–Wang theorem. □

Example. Consider the sequence

$$\left[10,\ 10,\ 9,\ 9,\ 8,\ 7,\ 6,\ 5,\ 4,\ 3,\ 2,\ 1\right].$$

Since $n = 12$ and $t = 10$, we have $\xi(n) = 9$. Also $t(2n - t + 1) \equiv 2(4)$, but $t > \xi(n)$. Therefore by Theorem 7, this sequence is not graphic. On the other hand it does not satisfy the Erdős–Gallai inequality when $k = 6$.

Theorem 8. *Let $G \in \mathcal{M}_{n,t}$. If $t \leq \xi(n)$, then*

$$|E(G)| \leq \left\lfloor \frac{t(2n - t + 1)}{4} \right\rfloor \tag{17}$$

with equality holding if and only if G realizes the sequence either (5) or (6).

Proof. Since $t \leq \xi(n)$, by Theorem 7 it follows that there exists a graph H in $\mathcal{M}_{n,t}$ which realizes the sequence either (5) or (6). Then $|E(G)| \leq |E(H)|$. If H realizes the sequence (5), then $|E(H)| = \frac{t(2n-t+1)}{4}$, otherwise $|E(H)| = \frac{t(2n-t+1)-2}{4}$. Therefore from the above, we get (17).

Moreover, if G does not realize either (5) or (6), then clearly the inequality in (17) is strict. Hence the theorem. □

* * * * *

Concluding this paper, we wish to point out an open problem.

We have studied the maximum size of maximally irregular graphs with given order and irregularity index (maximum degree). As shown above, the class of maximally irregular graphs of order n with irregularity index t is a large class of graphs. In [28] and [24], it was proven that if G is a maximally irregular triangle–free graph of order n, then the irregularity index t of G satisfies $t \leq \lfloor \frac{2n}{3} \rfloor$. Thus the following problems arises naturally: Establish an upper bound on the size of maximally irregular triangle–free graphs in terms of order and irregularity index. Characterize the degree sequence of a maximally irregular triangle–free graph with given order and irregularity index for which the size is maximum.

References

[1] H. Abdo, S. Brandt, D. Dimitrov, The total irregularity of a graph, *Discr. Math. Theor. Comput. Sci.* **16** (2014) 201–206.

[2] H. Abdo, N. Cohen, D. Dimitrov, Graphs with maximal irregularity, *Filomat* **28** (2014) 1315–1322.

[3] H. Abdo, D. Dimitrov, The total irregularity of graphs under graph operations, *Miskolc Math. Notes* **15** (2014) 3–17.

[4] H. Abdo, D. Dimitrov, The irregularity of graphs under graph operations, *Discuss. Math. Graph Theory* **34** (2014) 263–278.

[5] Y. Alavi, A. Boals, G. Chartrand, P. Erdős, O. Oellermann, k-path irregular graphs, *Congr. Numer.* **65** (1988) 201–210.

[6] Y. Alavi, G. Chartrand, F. R. K. Chung, P. Erdős, R. L. Graham, O. R. Oellermann, Highly irregular graphs, *J. Graph Theory* **11** (1987) 235–249.

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

[8] M. Albertson, D. Berman, Ramsey graphs without repeated degrees, *Congr. Numer.* **83** (1991) 91–96.

[9] M. Behzad, G. Chartrand, No graph is perfect, *Am. Math. Monthly* **74** (1967) 962–963.

[10] F. K. Bell, A note on the irregularity of graphs, *Lin. Algebra Appl.* **161** (1992) 45–54.

[11] N. L. Biggs, E. K. Lloyd, R. J. Wilson, *Graph Theory 1736 – 1936*, Clarendon Press, Oxford, 1976.

[12] G. Chartrand, P. Erdős, O. Oellermann, How to define an irregular graph, *College Math. J.* **19** (1988) 36–42.

[13] G. Chen, P. Erdős, C. Rousseau, R. Schelp, Ramsey problems involving degrees in edge–colored complete graphs of vertices belonging to monochromatic subgraphs, *Eur. J. Comb.* **14** (1993) 183–189.

[14] L. Collatz, U. Sinogowitz, Spektren endlicher Graphen, *Abh. Math. Sem. Univ. Hamburg* **21** (1957) 63–77.

[15] D. Cvetković, P. Rowlinson, On connected graphs with maximal index, *Publ. Inst. Math. Beograd* **44** (1988) 29–34.

[16] D. Dimitrov, R. Škrekovski, Comparing the irregularity and the total irregularity of graphs, *Ars Math. Contemp.* **9** (2015) 45–50.

[17] C. Elphick, P. Wocjan, New measures of graph irregularity, *El. J. Graph Theory Appl.* **2**(1) (2014) 52–65.

[18] P. Erdős, T. Gallai, Gráfok előírt fokú pontokkal, *Mat. Lapok* **11** (1960) 264–274.

[19] G. Fath–Tabar, Old and new Zagreb indices of graphs, *MATCH Commun. Math. Comput. Chem.* **65** (2011) 79–84.

[20] B. Furtula, I. Gutman, A forgotten topological index, *J. Math. Chem.* **53** (2015) 1184–1190.

[21] I. Gutman, P. Hansen, H. Mélot, Variable neighborhood search for extremal graphs 10. Comparison of irregularity indices for chemical trees, *J. Chem. Inf. Model.* **45** (2005) 222–230.

[22] A. Hamzeh, T. Réti, An analogue of Zagreb index inequality obtained from graph irregularity measures, *MATCH Commun. Math. Comput. Chem.* **72** (2014) 669–684.

[23] D. J. Kleitman, D. L. Wang, Algorithms for constructing graphs and digraphs with given valences and factors, *Discr. Math.* **6** (1973) 79–88.

[24] F. Liu, Z. Zhang, J. Meng, The size of maximally irregular graphs and maximally irregular triangle–free graphs, *Graphs Comb.* **30** (2014) 699–705.

[25] Z. Majcher, J. Michael, Degree sequence of highly irregular graphs, *Discr. Math.* **164** (1997) 225–236.

[26] Z. Majcher, J. Michael, Highly irregular graphs with extreme numbers of edges, *Discr. Math.* **164** (1997) 237–242.

[27] S. Mukwembi, A note on diameter and the degree sequence of a graph, *Appl. Math. Lett.* **25** (2012) 175–178.

[28] S. Mukwembi, On the maximally irregular graphs, *Bull. Malays. Math. Sci. Soc.* **36** (2013) 717–721.

[29] E. Ruch, I. Gutman, The branching extent of graphs, *J. Comb. Inf. System Sci.* **4** (1979) 285–295.