Graphs of prescribed order and size with maximal total irregularity

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Abstract

The total irregularity of a simple undirected graph G is defined as $\mathrm{irr}_t(G) = \frac{1}{2}\sum_{u,v \in V(G)} |d_G(u) - d_G(v)|$, where $d_G(u)$ denotes the degree of a vertex $u \in V(G)$. General graphs with maximal total irregularity were characterized in [2]. Here, we extend this result by characterizing graphs with maximal total irregularity and a fixed number of vertices and edges, both in the general and in the connected case. Since a connected graph with n vertices and m edges has cyclomatic number $c = m - n + 1$, the results presented here also generalize those of You, Yang, and You [27, 28], who characterized graphs with cyclomatic numbers 1 and 2 having maximal total irregularity. In addition, we reformulate the problem as a combinatorial optimization task and provide its solution in this context.

Keywords: the total irregularity of a graph, k-cyclic graphs.

1 Introduction and some related results

Let G be a simple undirected graph of order $n = |V(G)|$ and size $m = |E(G)|$. For $v \in V(G)$, the degree of v, denoted by $d_G(v)$, is the number of edges incident to v. G is *regular* if all its vertices have the same degree, otherwise, it is *irregular*. Several approaches have been proposed [8–19, 26] that characterize how irregular a given graph is. In this paper, we focus on the so-called *total irregularity* of a graph [2], defined as

$$\operatorname{irr}_t(G) = \frac{1}{2} \sum_{u,v \in V(G)} |d_G(u) - d_G(v)|. \tag{1}$$

The total irregularity is related to the *irregularity* of a graph, defined as $\operatorname{irr}(G) = \sum_{uv \in E(G)} |d_G(u) - d_G(v)|$. The latter measurement was introduced by Albertson [11] and investigated in several works [1, 23–25, 29, 30]. About the motivation of introducing total irregularity as a new irregularity measure, we refer an interested reader to [2]. Both measures, the irregularity of a graph and the total irregularity of a graph, depend only on one single parameter, namely the pairwise difference of vertex degrees. A comparison of irr and irr_t was considered in [21]. There, it was shown that $\operatorname{irr}_t(G) \leq n^2 \operatorname{irr}(G)/4$ and when G is a tree, then $\operatorname{irr}_t(G) \leq (n-2)\operatorname{irr}(G)$. Also, it was shown that among all trees of the same order, the star has the maximal total irregularity. The properties of the irregularity and the total irregularity under several graph operations and their comparison with several other irregularity measures were studied in [3–6, 20, 31].

In [2], graphs with maximal total irregularity were fully characterized and the upper bound on the total irregularity of a graph was presented. The structure of the graphs with maximal total irregularity is based on the so-called half-complete graphs [22]. A *half-complete* graph with n vertices is a graph that has $n-1$ different degrees. There are two such possible sets of degrees: $\{1, 2, \ldots, n-1\}$ and $\{0, 1, \ldots, n-2\}$, since a simple graph cannot contain vertices of degree 0 and $n-1$ at the same time. A simple induction proof verifies that for every n there is a unique graph with the respective set of degrees up to isomorphism. The graph with a vertex of degree $n-1$ is denoted by H_n and the graph with a vertex of degree 0 is its complement, denoted by $\overline{H}_n$ (see Figure **??** for an illustration). The graph H_n (resp. $\overline{H}_n$) can be obtained by labeling the vertices $v_1, \ldots, v_n$ and adding all edges $v_i v_j$ where $i + j \geq n + 1$ (resp. $i + j > n + 1$).

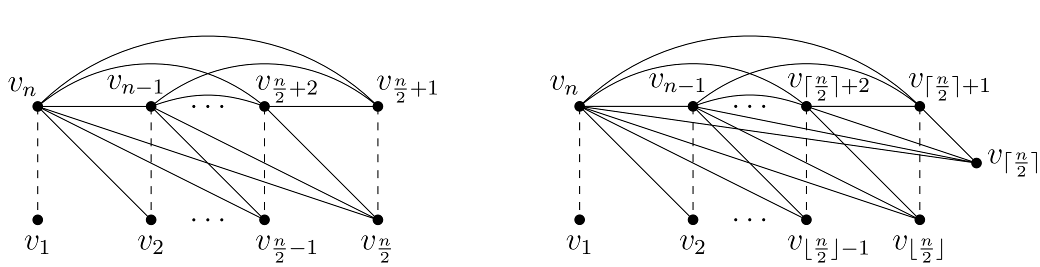


Figure 1: Graphs with maximal total irregularity H_n (with dashed edges) and $\overline{H}_n$ (without dashed edges) for even and odd n, respectively.

Take the graph H_n with vertices labeled as above and let $S = \{v_i v_j \mid i + j = n + 1\}$ (the set of dashed edges in Figure **??**). Then $\overline{H}_n = H_n - S$, $|E(\overline{H}_n)| = \lfloor n/2 \rfloor (\lceil n/2 \rceil - 1)$ and $|E(H_n)| = \lfloor n/2 \rfloor \lceil n/2 \rceil$.

Theorem 1.1 ([2]). *A graph G of order n has maximal total irregularity if and only if it is isomorphic to a graph $H_n - S'$, where $\emptyset \subseteq S' \subseteq S$.*

Corollary 1.1 ([2]). *For a simple undirected graph G with n vertices,*

$$\operatorname{irr}_t(G) \leq \begin{cases} \frac{1}{12}(2n^3 - 3n^2 - 2n) & n \textit{ even}, \\ \frac{1}{12}(2n^3 - 3n^2 - 2n + 3) & n \textit{ odd}. \end{cases}$$

Moreover, the bounds are sharp.

The *cyclomatic number* (or the *circuit rank*) of an undirected graph G is the minimum number of edges whose removal from G breaks all its cycles, making it into a tree or a forest. The cyclomatic number c can be expressed as $c = |E(G)| - |V(G)| + |C(G)|$, where $|C(G)|$ is the number of connected components of G. Since we are interested in connected graphs, we will assume that $|C(G)| = 1$. The graphs with cyclomatic numbers 1 and 2 are called unicyclic and bicyclic graphs, respectively. In [27, 28], the unicyclic and bicyclic graphs, respectively, with maximal total irregularity were determined. They are depicted in Figure 2. We refer the reader to [7] for more information on the total irregularity of cyclic graphs.

Figure 2: Unicyclic and bicyclic graphs with maximal total irregularity.

In this paper, we extend the results of [2] by providing a characterization of graphs with maximal total irregularity and a fixed number of edges, considering both connected and disconnected graphs. Since a connected graph with n vertices and m has the cyclomatic number $c = m - n + 1$, our result also generalizes the results from [27, 28], where the unicyclic and bicyclic graphs with maximal total irregularity were characterized.

A *universal vertex* in a graph is a vertex that is adjacent to every other vertex of the graph. The family of all graphs with of order n and size m is denoted by $\mathcal{G}_{n,m}$. Let G be a graph with $v_i v_j \in E(G)$, $v_l v_t \notin E(G)$. $G - v_i v_j$ denotes the graph obtained by deleting the edge $v_i v_j$ from G and $G + v_l v_t$ denotes the graph obtained by adding an edge $v_l v_t$ to G.

In the next section, we present preliminary results that will be used in Section 3, the graphs with fixed number of edges and maximal total irregularity are characterized. As a corollary, we obtain the sharp upper bound of the total irregularity of graphs with a fixed number of edges. In the last section, the underlying combinatorial problem will be presented.

2 Preliminary results

To characterize the graphs with maximal total irregularity and fixed number of edges, we will use the following two results.

Proposition 2.1. *Let G be a simple undirected graph and let $\overline{G}$ be its complement. Then,*

$$\mathrm{irr}_t(G) = \mathrm{irr}_t(\overline{G}).$$

Proof. Let G be a graph with vertex set $\{v_1, \ldots, v_n\}$. Then $d_{\overline{G}}(v_i) = n - 1 - d_G(v_i)$, $i = 1, \ldots, n$. The total irregularity of $\overline{G}$ is

$$\mathrm{irr}_t(\overline{G}) = \frac{1}{2} \sum_{u,v \in V(\overline{G})} |d_{\overline{G}}(u) - d_{\overline{G}}(v)| = \frac{1}{2} \sum_{u,v \in V(G)} \big|(n-1-d_G(u)) - (n-1-d_G(v))\big|$$

$$= \frac{1}{2} \sum_{u,v \in V(G)} |d_G(u) - d_G(v)| = \mathrm{irr}_t(G). \qquad \square$$

Lemma 2.1. *Let G be a graph with vertex set $\{v_1, \ldots, v_n\}$ such that $d(v_1) \geq d(v_2) \geq \cdots \geq d(v_n)$. Let $v_iv_j \notin E(G)$ and $v_kv_l \in E(G)$. If $i + j \leq k + l$, then*

$$\mathrm{irr}_t(G + v_iv_j - v_kv_l) \geq \mathrm{irr}_t(G).$$

Moreover, equality holds if $i + j = k + l$.

Proof. We may assume that $i < j$ and $k < l$. Consider first adding an edge v_iv_j to G. This increases all summands $d(v_i) - d(v_p)$ with $i < p$ and $p \neq j$ by one. If $i > p$ adding an edge v_iv_j decreases the summands $d(v_p) - d(v_i)$ by one or it increases them by one, if $d_G(v_p) = d_G(v_i)$. Similarly, all summands $d(v_j) - d(v_p)$ with $j < p$ are increased by one, while the summands $d(v_p) - d(v_j)$ for $j > p$ and $p \neq i$ are decreased by one or increased by one, if $d_G(v_p) = d_G(v_j)$.

Deleting an edge v_kv_l from G has the effect that all summands $d(v_p) - d(v_k)$ with $p < k$ are increased by one while the summands $d(v_k) - d(v_p)$ with $p > k$, $p \neq l$ are decreased by one (or increased by one, if $d_G(v_p) = d_G(v_k)$). All summands $d(v_p) - d(v_l)$ with $p < l$, $p \neq k$, are increased by one, while the summands $d(v_l) - d(v_p)$ with $p > l$, are decreased by one or increased by one, if $d_G(v_p) = d_G(v_l)$.

For $i < j$, $k < l$, and $i + j \leq k + l$, there are the following possible cases with respect to the cardinality of $V' = \{v_i, v_j, v_k, v_l\}$:

Case 1: $|V'| = 4$. In this case, due to the assumptions $i + j \leq k + l$, $i < j$ and $k < l$, there are four possibilities with respect to the position of the vertices v_i, v_j, v_k, and v_l: $i < j < k < l$, $i < k < j < l$, $i < k < l < j$ and $k < i < j < l$.

Subcase 1.1: $i < j < k < l$.

After adding an edge v_iv_j and deleting an edge v_kv_l, we have the following changes in the total irregularity related to the vertex v_i:

$$\sum_{p<i} (d(v_p) - d(v_i)) \geq -(i-1) \quad \text{and} \quad \sum_{p>i} (d(v_i) - d(v_p)) = n - i + 1.$$

Further changes of irr_t related to the vertices v_j, v_k and v_l are

$$\sum_{\substack{p<j\\ p\neq i}}(d(v_p)-d(v_j)) \geq -(j-2) \quad \text{and} \quad \sum_{p>j}(d(v_j)-d(v_p)) = n-j+2,$$

$$\sum_{\substack{p<k\\ p\neq i,j}}(d(v_p)-d(v_k)) = k-3 \quad \text{and} \quad \sum_{p>k}(d(v_k)-d(v_p)) \geq -(n-k-1),$$

and

$$\sum_{\substack{p<l\\ p\neq i,j,k}}(d(v_p)-d(v_l)) = l-4 \quad \text{and} \quad \sum_{p>l}(d(v_l)-d(v_p)) \geq -(n-l),$$

respectively. Thus, we have

$$\begin{aligned}\mathrm{irr}_t(G+v_iv_j-v_kv_l) &\geq \mathrm{irr}_t(G)-(i-1)+(n-i+1)-(j-2)+(n-j+2)\\ &\quad +(k-3)-(n-k-1)+(l-4)-(n-l)\\ &= \mathrm{irr}_t(G)+2(k+l-i-j).\end{aligned}$$

Together with the assumption $i<j<k<l$, it follows that $\mathrm{irr}_t(G+v_iv_j-v_kv_l) > \mathrm{irr}_t(G)$.

Subcase 1.2: $i<k<j<l$.

To avoid a repetition of similar arguments as in the previous case, here we just state the final relation between $\mathrm{irr}_t(G+v_iv_j-v_kv_l)$ and $\mathrm{irr}_t(G)$.

$$\begin{aligned}\mathrm{irr}_t(G+v_iv_j-v_kv_l) &\geq \mathrm{irr}_t(G)-(i-1)+(n-i+1)+(k-2)-(n-k)\\ &\quad -(j-3)+(n-j+1)+(l-4)-(n-l)\\ &= \mathrm{irr}_t(G)+2(k+l-i-j).\end{aligned}$$

Since $i<k<j<l$, we have that $\mathrm{irr}_t(G+v_iv_j-v_kv_l) > \mathrm{irr}_t(G)$.

Subcase 1.3: $i<k<l<j$.

Here, the changes of irr_t related to the vertices v_i, v_j, v_k and v_l are

$$\sum_{p<i}(d(v_p)-d(v_i)) \geq -(i-1) \quad \text{and} \quad \sum_{p>i}(d(v_i)-d(v_p)) = n-i+1,$$

$$\sum_{\substack{p<k\\ p\neq i}}(d(v_p)-d(v_k)) = k-2 \quad \text{and} \quad \sum_{p>k}(d(v_k)-d(v_p)) \geq -(n-k),$$

$$\sum_{\substack{p<l\\ p\neq i,k}}(d(v_p)-d(v_l)) = l-3 \quad \text{and} \quad \sum_{p>l}(d(v_l)-d(v_p)) \geq -(n-l+1),$$

and

$$\sum_{\substack{p<j\\ p\neq i,k,l}}(d(v_p)-d(v_j)) \geq j-4 \quad \text{and} \quad \sum_{p>j}(d(v_j)-d(v_p)) = n-j,$$

respectively. Thus, we have

$$\begin{aligned} \mathrm{irr}_t(G+v_iv_j-v_kv_l) &\geq \mathrm{irr}_t(G)-(i-1)+(n-i+1)+(k-2)-(n-k) \\ &\quad +(l-3)-(n-l+1)-(j-4)+(n-j) \\ &= \mathrm{irr}_t(G)+2(k+l-i-j). \end{aligned}$$

Since $i+j \leq k+l$, the claim of the lemma holds. The equality in $\sum_{p<i}(d(v_p)-d(v_i)) \geq -(i-1)$ holds when for every $p<i$ we have $d(v_p)>d(v_i)$. Also, $\sum_{p>k}(d(v_k)-d(v_p)) = -(n-k)$, if for every $p>k$ we have $d(v_k)>d(v_p)$, $\sum_{p>l}(d(v_l)-d(v_p)) = -(n-l+1)$ if for every $p>l$ the inequality $d(v_l)>d(v_p)$ holds, and $\sum_{\substack{p<j \\ p\neq i,k,l}}(d(v_p)-d(v_j)) = j-4$ if for every $p<j$ we have $d(v_p)>d(v_j)$. If in addition to the above mentioned conditions, $i+j=k+l$ holds, we have that $\mathrm{irr}_t(G+v_iv_j-v_kv_l)=\mathrm{irr}_t(G)$.

Subcase 1.4: $k<i<j<l$.
With similar arguments as in Subcase 1.3, we obtain that

$$\begin{aligned} \mathrm{irr}_t(G+v_iv_j-v_kv_l) &\geq \mathrm{irr}_t(G)+(k-1)-(n-k+1)-(i-2)+(n-i) \\ &\quad -(j-3)+(n-j+1)+(l-4)-(n-l) \\ &= \mathrm{irr}_t(G)+2(k+l-i-j), \end{aligned}$$

and that equality holds when $d(v_k)>d(v_p)$ for $p>k$, $d(v_i)<d(v_p)$ for $p<i$, $d(v_j)<d(v_p)$ for $p<j$, and $d(v_l)>d(v_p)$ for $p>l$.

Case 2: $|V'|=3$. In this case, there are three feasible possibilities.
Subcase 2.1: $i=k<j<l$.
Here, we have

$$\begin{aligned} \mathrm{irr}_t(G+v_iv_j-v_kv_l) &\geq \mathrm{irr}_t(G)-(j-1)+(n-j+1)+(l-2)-(n-l) \\ &= \mathrm{irr}_t(G)+2(l-j). \end{aligned}$$

From $j<l$, it follows that $\mathrm{irr}_t(G+v_iv_j-v_kv_l)>\mathrm{irr}_t(G)$.
Subcase 2.2: $i<j=k<l$.
We have

$$\begin{aligned} \mathrm{irr}_t(G+v_iv_j-v_kv_l) &\geq \mathrm{irr}_t(G)-(i-1)+(n-i+1)+(l-2)-(n-l) \\ &= \mathrm{irr}_t(G)+2(l-i). \end{aligned}$$

From $i<l$, we obtain $\mathrm{irr}_t(G+v_iv_j-v_kv_l)>\mathrm{irr}_t(G)$.
Subcase 2.3: $i<k<j=l$.
In this case, we have

$$\begin{aligned} \mathrm{irr}_t(G+v_iv_j-v_kv_l) &\geq \mathrm{irr}_t(G)-(i-1)+(n-i+1)+(k-2)-(n-k) \\ &= \mathrm{irr}_t(G)+2(k-i). \end{aligned}$$

Since $i < k$, it follows that $\mathrm{irr}_t(G + v_iv_j - v_kv_l) > \mathrm{irr}_t(G)$.

Case 3**:** $|V'| = 2$.
In this trivial case, $i = k$ and $j = l$, i.e., $v_iv_j = v_kv_l$, so there is no change of G and its total irregularity.

Notice that due to the assumptions $i+j \leq k+l$, $i < j$ and $k < l$ there are no further possible cases. □

3 Graphs of fixed order and size with maximal total irregularity

In the sequel, we assume that the vertices of the graphs are labeled such that $d(v_1) \geq d(v_2) \geq \cdots \geq d(v_n)$.

Proposition 3.1. *Let G_1 and G_2 be two graphs of order n and size m with maximal total irregularity. Then, for each edge $v_iv_j \in E(G_1)$ there is an edge $v_kv_l \in E(G_2)$ such that $i + j = k + l$.*

Proof. First, to every edge $v_iv_j \in E(G_1)$ assign an edge $v_kv_l \in E(G_2)$ if $i = k$ and $j = l$. Second, for the rest of the edges, we associate $v_iv_j \in E(G_1)$ and $v_kv_l \in E(G_2)$ if $i + j = k + l$. Finally, for the remaining edges, if any, we assign an arbitrary correspondence.

Now, assume that there is a pair of edges $v_iv_j \in E(G_1)$ and $v_kv_l \in E(G_2)$ such that $i + j \neq k + l$. We may also assume that $i + j < k + l$. Delete the edge v_kv_l and add the edge v_iv_j in G_2. By Lemma 2.1, we have that $\mathrm{irr}_t(G_2 + v_iv_j - v_kv_l) > \mathrm{irr}_t(G_2)$, which is a contradiction to the initial assumption that G_2 is a graph with maximal total irregularity. □

By Lemma 2.1 and Proposition 3.1, the following two immediate consequences follow.

Corollary 3.1. *Let G_1 and G_2 be two graphs of order n and size m with maximal total irregularity. Then, $\sum_{u_iu_j \in E(G_1)}(i + j) = \sum_{v_kv_l \in E(G_2)}(k + l)$.*

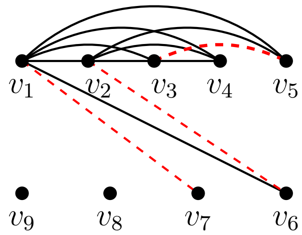
Corollary 3.2. *Let G be a graph with maximal total irregularity among graphs of order n and size m. Then, $G \in \mathrm{argmin}_{H \in \mathcal{G}_{n,m}} \sum_{u_iv_j \in E(H)}(i + j)$.*

For fixed n and a parameter k with $3 \leq k \leq n + 1$, let G_k be the graph with the vertex set $V(G_k) = \{v_1, v_2, \ldots, v_n\}$ and the edge set $E(G_k) = E_{<k}(G_k) \cup E_{=k}(G_k)$, where $E_{<k}(G_k) := \{v_iv_j : i + j < k\}$ and $E_{=k}(G_k) := \{v_iv_j : i + j = k\}$.

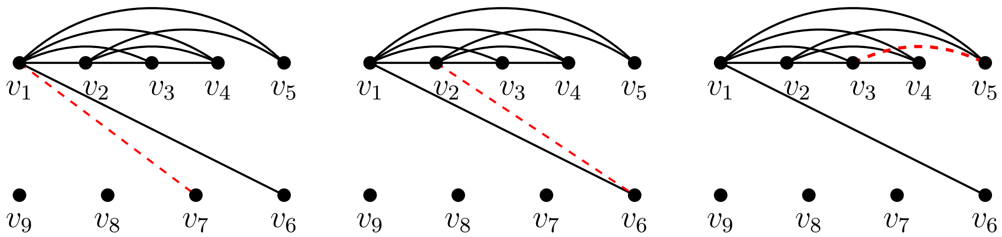
For an illustration see the graph G_8 with $n = 9$ vertices in Figure 3a.

For a given $m \leq \binom{n}{2}/2$, we choose as the largest parameter k such that $|E_{<k}(G_k)| \leq m$. For $n = 9$ and $m = 10$, we would thus choose $k = 8$, as in Figure 3(a). Let $r := m - |E_{<k}(G_k)|$.

We now define the family $\mathcal{G}_k^r$ of graphs of order n and size m as follows: $\mathcal{G}_k^r$ consists of all graphs G with $V(G) = V(G_k)$ and $E(G) = E_{<k}(G_k) \cup E'_{=k}(G_k)$, where $E'_{=k}(G_k)$ is an arbitrary subset of $E_{=k}(G_k)$ with cardinality r. Figure 3b shows the family of graphs $\mathcal{G}_8^1$.



(a) G_8



(b) $\mathcal{G}_8^1$

Figure 3: (a) The graph G_8 obtained for $n = 9$ and $m = 10$. G_8 has 9 edges. The edges $E_{<k}(G_8)$ are depicted in black, while the edges $E_{=k}(G_8)$ are depicted in red dashed. (b) The family of graphs $\mathcal{G}_8^1$.

Theorem 3.1. *A simple undirected graph G has maximal total irregularity among all graphs with n vertices and m edges if and only if $G \in \mathcal{G}_k^r$.*

Proof. By the definition of $\mathcal{G}_k^r$ and Corollary 3.2 every $G \in \mathcal{G}_k^r$ has maximal total irregularity. To show that the other direction of the equivalence holds, we assume that there is a graph $H \notin \mathcal{G}_k^r$ with maximal total irregularity. Since $H \notin \mathcal{G}_k^r$, considering the definition of $\mathcal{G}_k^r$, there must be an edge $v_k v_l \in E(H)$ and two not adjacent vertices $v_i, v_j \in V(H)$ such that $i + j > k + l$. By Lemma 2.1, $\mathrm{irr}_t(H + v_i v_j - v_k v_l) \geq \mathrm{irr}_t(H)$, which is a contradiction. □

The following result helps us to determine the maximal total irregularity.

Proposition 3.2. $|E_{<k}(G_k)| = (\lfloor \frac{k}{2} \rfloor - 1)(\lceil \frac{k}{2} \rceil - 1)$ *and* $|E_{=k}(G_k)| = \lceil \frac{k}{2} \rceil - 1$.

Proof. Consider an edge $v_i v_j \in E_{<k}(G_k)$. From the definition of $E_{<k}(G_k)$, we have that $i + j < k$. We may assume that $i < j$. From these two constraints, it follows that $i \in \{1, \ldots, \lfloor \frac{k}{2} \rfloor - 1\}$. The neighbors v_j of v_i in $E_{<k}$ with $j > i$ are $v_{i+1}, v_{i+2}, \ldots, v_{k-i-1}$, and their number is $k - 2i - 1$. Consequently, the total number of edges in $E_{<k}(G_k)$ is

$$|E_{<k}(G_k)| = \sum_{i=1}^{\lfloor \frac{k}{2} \rfloor - 1} (k - 2i - 1) = \left(\left\lfloor \frac{k}{2} \right\rfloor - 1 \right) \left(\left\lceil \frac{k}{2} \right\rceil - 1 \right).$$

Now, we determine the cardinality of the set $E_{=k}(G_k)$. Consider an edge $v_iv_j \in E_{=k}(G_k)$. Due to constraints $i+j=k$ and $i<j$, it follows that $i \in \{1,\ldots,\lceil \frac{k}{2} \rceil - 1\}$. For each i, there is exactly one edge v_iv_j in $E_{=k}(G_k)$. Thus,

$$|E_{=k}(G_k)| = \sum_{i=1}^{\lceil \frac{k}{2} \rceil - 1} 1 = \left\lceil \frac{k}{2} \right\rceil - 1. \qquad \square$$

Next, we determine the value of the maximal total irregularity.

Proposition 3.3. *Let G be a graph in $\mathcal{G}_{n,m}$ with maximum total irregularity, for $m \leq \binom{n}{2}/2$. Then,*

$$\mathrm{irr}_t(G) = \begin{cases} \frac{1}{12}(k-2)\left(k(6n+19) - 4k^2 - 12(n+2)\right) + 2r(k+1) & \text{if } n \text{ is even}, \\ \frac{1}{12}\left(k^2 - 4k + 3\right)(6n - 4k + 11) + 2r(k+1) & \text{if } n \text{ is odd}. \end{cases}$$

Proof. Let G_k be a graph with n vertices as defined above. Recall that $E(G_k) = E_{<k}(G_k) \cup E_{=k}(G_k)$ with $E_{<k}(G_k) = \{v_iv_j : i+j<k\}$ and $E_{=k}(G_k) = \{v_iv_j : i+j=k\}$. We partition the vertex set of G_k into $V_1 = \{v_i : 1 \leq i \leq \lceil \frac{k}{2} \rceil - 1\}$, $V_2 = \{v_i : \lceil \frac{k}{2} \rceil - 1 < i < k-1\}$, and $V_3 = \{v_i : i \geq k-1\}$. Further, we examine the graph H with $V(H) = V(G_k)$ and $E(H) = E_{<k}(G_k)$.

Firstly, consider the case when a vertex v_i is in V_1. In the graph H, there are exactly $i-1$ adjacent vertices to v_i, whose indices are smaller than i and $k-2i-1$ vertices, whose indices are larger than i. Thus, a vertex v_i in V_1 has a degree $k-i-2$. In the case when v_i is in V_2, there is no adjacent vertex to v_i in H, whose index j is larger than i, due to the constraints $\lceil \frac{k}{2} \rceil - 1 < i < k-1$, $i+j<k$ and $i<j$, However, there are $k-i-1$ adjacent vertices to v_i, whose indices are smaller than i. Therefore, a vertex v_i in V_2 has a degree $k-i-1$. Similarly, we can conclude that a vertex v_i in V_3 does not have any adjacent vertices, i.e., it has degree 0. Summarized, the degrees of the vertices in H are as follows:

$$d_H(v_i) = \begin{cases} k-i-2 & \text{if } v_i \in V_1(G_k), i.e., 1 \leq i \leq \lceil \frac{k}{2} \rceil - 1, \\ k-i-1 & \text{if } v_i \in V_2(G_k), i.e., \lceil \frac{k}{2} \rceil - 1 < i < k-1, \\ 0 & \text{if } v_i \in V_3(G_k), i.e., i \geq k-1. \end{cases} \tag{2}$$

Then, the total irregularity of H is

$$\begin{aligned} \mathrm{irr}_t(H) &= \sum_{i<j}(d_H(v_i) - d_H(v_j)) = \sum_{i=1}^{n-1}\sum_{j=i+1}^{n}(d_H(v_i) - d_H(v_j)) \\ &= \sum_{v_i \in V_1(H)}\sum_{v_j \in V_1(H)}(d_H(v_i) - d_H(v_j)) + \sum_{v_i \in V_1(H)}\sum_{v_j \in V_2(H)}(d_H(v_i) - d_H(v_j)) \\ &+ \sum_{v_i \in V_1(H)}\sum_{v_j \in V_3(H)}(d_H(v_i) - d_H(v_j)) + \sum_{v_i \in V_2(H)}\sum_{v_j \in V_2(H)}(d_H(v_i) - d_H(v_j)) \\ &+ \sum_{v_i \in V_2(H)}\sum_{v_j \in V_3(H)}(d_H(v_i) - d_H(v_j)) + \sum_{v_i \in V_3(H)}\sum_{v_j \in V_3(H)}(d_H(v_i) - d_H(v_j)) \end{aligned}$$

$$= \sum_{i=1}^{\lceil \frac{k}{2} \rceil -1} \sum_{j=i+1}^{\lceil \frac{k}{2} \rceil -1} ((k-i-2)-(k-j-2)) + \sum_{i=1}^{\lceil \frac{k}{2} \rceil -1} \sum_{j=\lceil \frac{k}{2} \rceil}^{k-2} ((k-i-2)-(k-j-1))$$

$$+ \sum_{i=1}^{\lceil \frac{k}{2} \rceil -1} \sum_{j=k-1}^{n} ((k-i-2)-0) + \sum_{i=\lceil \frac{k}{2} \rceil}^{k-2} \sum_{j=i+1}^{k-2} ((k-i-1)-(k-j-1))$$

$$+ \sum_{i=\lceil \frac{k}{2} \rceil}^{k-2} \sum_{j=k-1}^{n} ((k-i-1)-0) + \sum_{i=k-1}^{n-1} \sum_{j=i+1}^{n} (0-0)$$

$$= \frac{1}{6}(n+2k+3)(n-k-1)(n-k-2) - n\left\lfloor \frac{n-k-1}{2} \right\rfloor + \left\lfloor \frac{n-k-1}{2} \right\rfloor^2$$

$$= \frac{1}{6}\left(6\left\lceil \tfrac{k}{2} \right\rceil(2k-n-2) - 6\left\lceil \tfrac{k}{2} \right\rceil^2 - 2k^3 + 3k^2(n+3) - k(9n+25) + 12(n+2)\right)$$

or in more explicit terms,

$$\mathrm{irr}_t(H) = \begin{cases} \frac{1}{12}(k-2)\left(k(6n+19) - 4k^2 - 12(n+2)\right), & \text{if } k \text{ is even} \\ \frac{1}{12}\left(k^2-4k+3\right)(6n-4k+11), & \text{if } k \text{ is odd} \end{cases}$$

Consider now the graph G_k^r obtained by adding r edges from $E_{=k}(G_k)$ to H. Thus, H can be extended to G_k^r in $\binom{|E_{=k}(G_k)|}{r}$ different ways, obtaining $\binom{|E_{=k}(G^k)|}{r}$ non-isomorphic graph with n vertices and $|E_{<k}(G_k)| + r$ edges. For an edge $v_iv_j \in E_{=k}(G_k)$, $i < j$, we have $1 \leq i \leq \lceil \frac{k}{2} \rceil - 1$, and $\lceil \frac{k}{2} \rceil \leq j \leq n-k-1$. From the above characterization of the degrees of the vertices of H, we have that $d_H(v_1) > d_H(v_2) > \cdots > d_H(v_{\lceil \frac{k}{2} \rceil -1}) = d_H(v_{\lceil \frac{k}{2} \rceil}) > \cdots > d_H(v_n)$ — we have everywhere a strict inequality except between $d_H(v_{\lceil \frac{k}{2} \rceil -1})$ and $d_H(v_{\lceil \frac{k}{2} \rceil})$, where equality holds. After adding an edge or up to r edges from $E_{=k}(G_k)$ to H, the degree of a vertex can be increased by at most one, and thus, the order of the degrees of vertices remains unchanged. After adding an edge $v_iv_j \in E_{=k}(G_k)$ to H the total irregularity decreases by $i-1+j-2$, since there are $i-1$ vertices with smaller index than v_i, and $j-2$ vertices with smaller index than j, different from i. Similarly, after adding an edge v_iv_j the total irregularity increases by $n-i-1+n-j$. Therefore, the total irregularity of G_k^r is

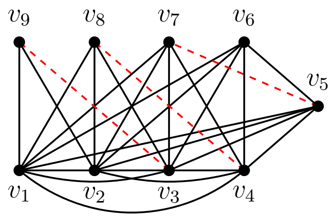
$$\begin{aligned} \mathrm{irr}_t(G_k^r) &= \mathrm{irr}_t(H) + r(-(i-1) + (n-i-1) - (j-2) + (n-j)) \\ &= \mathrm{irr}_t(H) + 2r(n-i-j+1) \\ &= \mathrm{irr}_t(H) + 2r(k+1). \end{aligned}$$

□

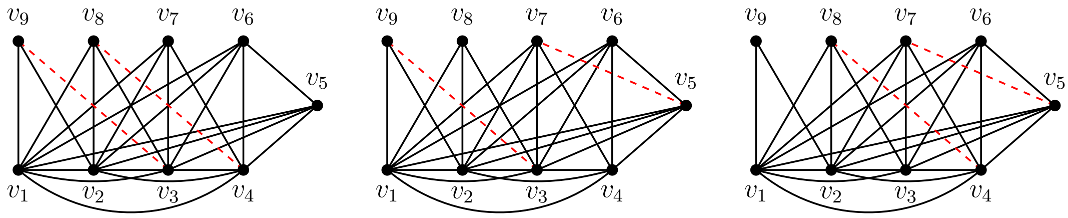
4 Extensions

A simple graph with n vertices can have $0 \leq m \leq \binom{n}{2}$ edges. By Proposition 2.1, a graph and its complement graph have the same total irregularity. It follows, that if a graph G

of order n and size m has maximal total irregularity, then a graph of the same order n and size $\binom{n}{2} - m$ with maximal total irregularity must be the complement graph of G. For an illustration see the graphs in Figure 4(b), which have maximal total irregularity among graphs of order 9 and size 26. They are complements of the graphs depicted in Figure 3(b), which have maximal total irregularity among graphs of order 9 and size 10.



(a) G_{12}



(b) $\mathcal{G}_{12}^2$

Figure 4: (a) The graph G_{12} obtained for $n = 9$ and $m = 26$. The parameter $k = 12$ and the edges set of G_{12} are uniquely determined as it was explained in the previous section. (b) The family of graphs $\mathcal{G}_{12}^2$ derived from the graph G_{12} ($r = 2$) with maximal total irregularity among all graphs of order 9 and size 26. Observe that each graph of $\mathcal{G}_{12}^2$ is a complement of a graph from $\mathcal{G}_8^1$ depicted in Figure 3(b). All graphs from $\mathcal{G}_{12}^2$ and $\mathcal{G}_8^1$ have total irregularity of 84.

As a consequence, to characterize graphs with maximal total irregularity of a given order n, it is sufficient to consider the graphs of order n and size $m \leq \frac{1}{2}\binom{n}{2}$. This leads to the same graphs as those characterized by Theorem 1.1.

4.1 Corresponding combinatorial problem

Due to Corollary 3.2, the problem of characterizing graphs with maximal total irregularity among all graphs with n vertices and m edges can be reformulated as the following problem: Find m different pairs of positive integers (i, j), $i < j < n$, such that the sum $i + j$ over all pairs is minimal. The number of ways to choose such m pairs (i, j) is the same as the number of graphs with maximal total irregularity.

For example, consider the problem of finding all sets of $m = 10$ pairs of positive integers (i, j), $i < j < n = 9$ such that the sum of $i + j$ over all pairs is minimal. The solution is illustrated in Tabel 1(a). The first 9 pairs are colored blue and they form the set $E_{<k} = \{(1,2),(1,3),(1,4),(1,5),(1,6),(2,3),(2,4),(2,5),(3,4)\}$. There are three possibilities for the tenth pair, which belongs to the column covered with pink stripes and they form the set $E_{=k} = \{(1,7),(2,6),(3,5)\}$. Thus the possible solutions are $E_{<k} \cup \{(1,7)\}, E_{<k} \cup \{(2,6)\}, E_{<k} \cup \{(3,5)\}$. Observe that each of these solutions corresponds to one of the three graphs from Figure 3(b), the graphs of order 9 with 10 edges and maximal total irregularity. This is due to the bijection between the above pairs (i,j) and the edges $v_i v_j$ of those graphs.

Similarly, the solution to the problem of finding all sets of $m = 26$ pairs of positive integers (i,j), $i < j < n = 9$ such that the sum of $i+j$ over all pairs is minimal is illustrated in Tabel 1(b). The first 24 pairs are colored blue and they form the set $\overline{E_{<k}} = \{(1,2),\ldots,(1,9),(2,3),\ldots,(2,9),(3,4),\ldots,(3,8),(4,5), cdots,(4,7),(5,6)\}$. There are three possibilities for the last two pairs, which belong to the column covered with pink stripes and they form the set $\overline{E_{=k}} = \{(3,9),(4,8),(5,7)\}$. Thus the possible solutions are $\overline{E_{<k}} \cup \{(3,9),(4,8)\}, \overline{E_{<k}} \cup \{(3,9),(5,7)\}, \overline{E_{<k}} \cup \{(4,8),(5,7)\}$. These solutions correspond to the three graphs from Figure 4(b).

(1,2)	(1,3)	(1,4)	(1,5)	(1,6)	(1,7)	(1,8)	(1,9)	(2,9)	(3,9)	(4,9)	(5,9)	(6,9)	(7,9)	(8,9)
		(2,3)	(2,4)	(2,5)	(2,6)	(2,7)	(2,8)	(3,8)	(4,8)	(5,8)	(6,8)	(7,8)		
				(3,4)	(3,5)	(3,6)	(3,7)	(4,7)	(5,7)	(6,7)				
						(4,5)	(4,6)	(5,6)						

(a) $n = 9,\ m = 10$

(1,2)	(1,3)	(1,4)	(1,5)	(1,6)	(1,7)	(1,8)	(1,9)	(2,9)	(3,9)	(4,9)	(5,9)	(6,9)	(7,9)	(8,9)
		(2,3)	(2,4)	(2,5)	(2,6)	(2,7)	(2,8)	(3,8)	(4,8)	(5,8)	(6,8)	(7,8)		
				(3,4)	(3,5)	(3,6)	(3,7)	(4,7)	(5,7)	(6,7)				
						(4,5)	(4,6)	(5,6)						

(b) $n = 9,\ m = \binom{n}{2} - 10 = 26$

Table 1: An illustration of the solution to the problem of finding all sets of m pairs of positive integers (i,j), $i < j < n = 9$, such that the sum $i+j$ over all pairs is minimal: (a) $m = 10$ and (b) $m = 26$.

4.2 Connected graphs

Up to this point, we have considered graphs of given order and size without imposing any structural constraints.

By the results obtained so far, a graph with maximal total irregularity is not necessarily connected. For example, among all graphs of order n and size n or $n+1$, those with maximal total irregularity are disconnected.

The minimal number of edges m that guarantees that a general graph with maximal total irregularity is connected can be determined as follows.

Firstly, for a graph in the family $\mathcal{G}_k^r$ to be connected, it must contain an edge incident to v_n, and therefore $k \geq n+1$.

Thus, the sets $E_{<k}(G_k)$ and $E_{=k}(G_k)$, introduced above and used to define the family $\mathcal{G}_k^r$, are in this case given by:

$$E_{<k}(G_{n+1}) = \{v_i v_j \colon i+j < n+1\}, \quad E_{=k}(G_{n+1}) = \{v_i v_j \colon i+j = n+1\},$$

with $r=1$. By Proposition 3.2, we have

$$|E_{<k}(G_{n+1})| = \left(\left\lfloor \frac{n+1}{2} \right\rfloor - 1\right)\left(\left\lceil \frac{n+1}{2} \right\rceil - 1\right),$$

and

$$|E_{=k}(G_{n+1})| = \left\lceil \frac{n+1}{2} \right\rceil - 1.$$

In $E_{<k}(G_{n+1})$, the vertex v_1 is almost universal: It is connected to every other vertex except v_n. To make this graph connected, it is sufficient to add one edge: the edge $v_1 v_n \in E_{=k}(G_{n+1})$. However, if we add any of the other edges of $E_{=k}(G_{n+1})$, we would leave v_n isolated. Omitting $v_1 v_n$ is possible as long as

$$m < |E_{<k}(G_{n+1})| + |E_{=k}(G_{n+1})| = \left(\left\lfloor \frac{n+1}{2} \right\rfloor + 1\right)\left(\left\lceil \frac{n+1}{2} \right\rceil - 1\right),$$

We summarize the conclusion of this argument as follows:

- For $m \leq \left(\left\lfloor \frac{n+1}{2} \right\rfloor - 1\right)\left(\left\lceil \frac{n+1}{2} \right\rceil - 1\right)$, none of the graphs with maximum total irregularity are connected.
- In the range $\left(\left\lfloor \frac{n+1}{2} \right\rfloor - 1\right)\left(\left\lceil \frac{n+1}{2} \right\rceil - 1\right) < m < \left(\left\lfloor \frac{n+1}{2} \right\rfloor + 1\right)\left(\left\lceil \frac{n+1}{2} \right\rceil - 1\right)$, some graphs are connected and some are disconnected.
- For $m \geq \left(\left\lfloor \frac{n+1}{2} \right\rfloor + 1\right)\left(\left\lceil \frac{n+1}{2} \right\rceil - 1\right)$, all graphs with maximum total irregularity are connected.

Imposing connectedness as a constraint. If we want to maximize the total irregularity *among the connected graphs*, we must slightly modify our approach. The following result provides a key step in this direction.

Proposition 4.1. *Let G be a connected graph of given order n and size m with maximal total irregularity. Then G has a universal vertex.*

Proof. As before, we assume that the vertices of G are labeled such that $d(v_1) \geq d(v_2) \geq \cdots \geq d(v_n)$. Suppose, for contradiction, that v_1 is not a universal vertex. Then there exists a vertex v_j that is not adjacent to v_1. Since G is connected, v_j must be adjacent to at least one other vertex, say v_i.

Now, construct a new graph G' by deleting the edge v_iv_j and adding the edge v_1v_j. By Lemma 2.1, $\operatorname{irr}_t(G') > \operatorname{irr}_t(G)$, which contradicts the assumption that G has maximal total irregularity. □

Knowing that $d(v_1) = n - 1$, we conclude that the contribution of the $n - 1$ pairs involving v_1 to the total irregularity is fixed: Since overall sum of the degrees is fixed ($2m$), the contribution $\sum_{i=2}^{n}(d(v_1) - d(v_i))$ has a fixed value. Moreover, the irregularity $|d(v_i) - d(v_j)|$ of the remaining pairs is not affected by the presence or absence of the universal vertex v_1. Thus, in order to optimize the total irregularity, it suffices to look at the graph $G - \{v_1\}$.

We conclude that any extremal *connected* graph with maximal total irregularity must consist of a general extremal graph on $n-1$ vertices with $m-n+1$ edges, together with an added universal vertex.

To formalize this construction, let $\mathcal{G}_k^r$ denote the family of extremal graphs as defined earlier. We define the family $\mathcal{C}_k^r$ of simple connected graphs as

$$\mathcal{C}_k^r = \{G\colon G = G' \cup \{v_1v_i : 2 \le i \le n\},\ G' \in \mathcal{G}_k^r,\ V(G') = \{v_2, \dots, v_n\}\},$$

where G' is a graph on $n - 1$ vertices, and the vertex v_1 is universal in G.

Theorem 4.1. *A graph G has maximal total irregularity among the simple connected undirected graph withs n vertices and m edges if and only if $G \in \mathcal{C}_k^r$.*

A connected graph with n vertices and m edges has cyclomatic number $c = m-n+1$. Thus, the results of You, Yang, and You [27, 28], where the unicyclic graphs ($c = 1$) and the bicyclic graphs ($c = 2$) with maximal total irregularity were characterized (see Figure 2), are special cases of the characterization presented here.

4.3 Independent Confirmation of Results

According to Corollary 3.2, the optimal graph consists of the m edges v_iv_j that minimize the sum of the terms $i+j$, *under the constraint* that the vertices $v_1, v_2, \dots, v_n$ are ordered by decreasing degree. It is easy to choose the m edges that minimize this sum when this extra constraint is relaxed: Simply sort all pairs (i, j) with $1 \le i < j \le n$ in increasing order by $i + j$, and select the m pairs with the smallest sums. It turns out (*a posteriori*, so-to-speak), that this selection of edges produces a graph G_m that fulfills the extra constraint about the ordering of the degrees. Therefore it is the optimum even *with the constraint*.

If the value $i + j$ for last included edge v_iv_j in G_m is $i + j = k$, then G_m includes all edges with $i + j < k$, and some edges with $i + j = k$.

Lemma 4.1. *Let $n \in \mathbb{N}$, and let $3 \le k \le 2n - 1$. Let G be a graph with vertex set $\{v_1, v_2, \dots, v_n\}$, consisting of all edges v_iv_j with $i \ne j$ and $i + j < k$, and* some *edges v_iv_j with $i \ne j$ and $i + j = k$. Then the degrees are weakly decreasing:*

$$d(v_1) \ge d(v_2) \ge \cdots \ge d(v_n)$$

Proof. Let us compare the degrees of v_i and v_{i+1}. If $k \le i$, then v_i and v_{i+1} have no neighbors, and there is nothing to prove. Thus we assume for the remainder of the proof that $k \ge i+1$.

We first prove the statement for the "pure" case that *all* edges with $i+j=k$ are included. We write $[a]$ for the set $\{1,2,\dots,a\}$. Then the index set of the neighbors of v_i is $[k-i]\setminus\{i\}$. Since $k-i \ge 1$, $[k-i]$ is nonempty, and the set $[k-(i+1)]$ has one element less than $[k-i]$. Removing one element i or $i+1$ to obtain the correct neighbor sets $[k-i]\setminus\{i\}$ and $[k-(i+1)]\setminus\{i+1\}$ cannot decrease the difference in size by more than 1. Thus $d(v_i) \ge d(v_{i+1})$. Equality holds if $[k-i]$ loses one element and $[k-(i+1)]$ doesn't, which happens if $i \in [k-i]$ and $i+1 \notin [k-(i+1)]$. Equivalently, $i \le k-i$ and $i+1 > k-i-1$, which can be rewritten as

$$k-1 \le 2i \le k. \tag{3}$$

Thus, we have established strict inequality $d(v_i) > d(v_{i+1})$, unless (3) holds.

Now we proceed to the general case, removing some of the edges with $i+j=k$. These edges form a matching, and hence, removing some of them decreases any degree by at most 1. As a consequence, the case where we had strict inequality before the removal is settled: The worst thing that can happen is that the strict inequality $d(v_i) > d(v_{i+1})$ is weakened to $d(v_i) \ge d(v_{i+1})$.

The case where (3) holds and $d(v_i) = d(v_{i+1})$ before the removal is split into two subcases:

(a) k is even, and $i = k/2$. In this case, the pair (i,j) with $i+j=k$ is the pair (i,i), which does not correspond to an edge. Thus, no edge incident to v_i is removed, and the degree $d(v_i)$ is unchanged, while $d(v_{i+1})$ can only decrease.

(b) k is odd, and $i = (k-1)/2$. In this case the pair (i,j) with $i+j=k$ is the pair $(i,i+1)$, and the corresponding edge is incident to both i and $i+1$. When this edge is removed, both degrees $d(v_i)$ and $d(v_{i+1})$ decrease simultaneosly by 1; other edges that are removed affect neither $d(v_i)$ nor $d(v_{i+1})$. □

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