# On Irregularity of Graphs

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**Abstract.** The graph's irregularity is the sum of the absolute values of the differences of degrees of pairs of adjacent vertices in the graph. We provide various upper bounds for the irregularity of a graph, especially for $K_{r+1}$-free graphs, where $K_{r+1}$ is a complete graph on $r+1$ vertices, and trees and unicyclic graphs of given number of pendant vertices.

**Keywords:** irregularity, $K_{r+1}$-free graph, tree, unicyclic graph, pendant vertex

## 1 Introduction

Let $G$ be a simple graph with vertex set $V(G)$ and edge set $E(G)$. The neighborhood of a vertex $u$ is the set of vertices adjacent to $u$ in $G$, denoted by $N_G(u)$. The degree of a vertex $u$ in $G$ is $d_G(u) = |N_G(u)|$. For simplicity, we also use $d_u$ instead of $d_G(u)$ if $G$ is understood. The irregularity of the graph $G$ is defined as [2]

$$\operatorname{irr}(G) = \sum_{uv \in E(G)} |d_u - d_v|.$$

Albertson [2] provided upper bounds for the irregularity of general, bipartite and triangle-free graphs, in particular, for a graph $G$ with $n$ vertices, it was shown that $\operatorname{irr}(G) < \frac{4n^3}{27}$ and that this bound can be approached arbitrarily closely. Hansen and Mélot [7] found a tight upper bound for the irregularity in terms of the numbers of vertices and edges, and it was shown that the extremal graphs are a particular class of split graphs (which consist of a clique, an independent set and some edges joining a vertex in the clique to a vertex in the independent set). Recently, Henning and Rautenbach [8] determined the structure of bipartite graphs having maximum possible irregularity with given cardinalities of the partite sets and given number of edges. Gutman *et al.* [6] characterized the chemical trees (trees with maximum degree at most four) having maximum possible irregularity. It was noted in [6] that the irregularity, which was called the Albertson index in [6], is a usable molecular structure descriptor both for descriptive purposes and quantitative structure-activity relationship (QSAR) and quantitative structure-property relationships (QSPR) studies.

In this paper, we provide various upper bounds for the irregularity of a graph, especially for $K_{r+1}$-free graphs, where $K_{r+1}$ is a complete graph on $r+1$ vertices, and trees and unicyclic graphs of given number of pendant vertices.

# 2 Irregularity of General Graphs

Let $K_{s,t}$ be the complete bipartite graph with two partite sets having $s$ and $t$ vertices, respectively.

We need an auxiliary graph invariant for a graph $G$: $Z(G) = \sum_{u\in V(G)} d_u^2$. It emerges in [3, 4, 5, 10] and is called the first Zagreb index in chemical graph theory, see, e.g., [13]. First we give a connection between irr$(G)$ and $Z(G)$.

**Theorem 1** *Let $G$ be a graph with $n$ vertices and $m$ edges. Then*

$$irr(G) \le \sqrt{m\,[nZ(G) - 4m^2]}$$

*with equality if and only if the degree of all vertices not adjacent to $u$ is equal to $d_u$ for any $u \in V(G)$ and $|d_u - d_v| = |d_x - d_y|$ for any $uv$, $xy \in E(G)$.*

**Proof.** By the definition of the irregularity and the Cauchy–Schwarz inequality,

$$\mathrm{irr}(G) = \sum_{uv\in E(G)} |d_u - d_v| \le \sqrt{m \sum_{uv\in E(G)} (d_u - d_v)^2}$$

with equality if and only if $|d_u - d_v| = |d_x - d_y|$ for any $uv$, $xy \in E(G)$. Note that

$$\begin{aligned}
\sum_{uv\in E(G)} (d_u - d_v)^2 &= \frac{1}{2} \sum_{u\in V(G)} \sum_{v\in N_G(u)} (d_u - d_v)^2 \\
&\le \frac{1}{2} \sum_{u\in V(G)} \sum_{v\in V(G)} (d_u - d_v)^2 \\
&= \frac{1}{2} \sum_{u\in V(G)} \sum_{v\in V(G)} (d_u^2 + d_v^2) - \sum_{u\in V(G)} \sum_{v\in V(G)} d_u d_v \\
&= nZ(G) - 4m^2
\end{aligned}$$

with equality if and only if the degree of all vertices not adjacent to $u$ is equal to $d_u$ for any $u \in V(G)$. Now the theorem follows easily. □

By Theorem 1, we may get upper bounds for irr$(G)$ from upper bounds for $Z(G)$. As examples, some of them are listed below:

(i) Let $G$ be a graph with $n$ vertices and $m \geq 1$ edges. Then [5, 10]

$$Z(G) \leq m\left(\frac{2m}{n-1} + n - 2\right)$$

with equality if and only if $G \cong K_{1,n-1}$, $K_n$, or $K_1 \cup K_{n-1}$. Thus

$$\mathrm{irr}(G) \leq m\sqrt{\frac{(n-2)\left[n(n-1) - 2m\right]}{n-1}}$$

with equality if and only if $G \cong K_{1,n-1}$ or $K_n$.

(ii) Let $G$ be a graph with $n$ vertices, $m$ edges, maximum degree $\Delta$ and minimum degree $\delta$. Then [4, 3]

$$Z(G) \leq \frac{2m\left[2m + (n-1)(\Delta - \delta)\right]}{n + \Delta - \delta}$$

with equality if and only if $G$ is a regular graph, $G \cong (n - \Delta - 1)K_1 \cup K_{\Delta+1}$, or $G \cong B_{n,t}$ for $1 \leq t \leq n-1$, where $B_{n,t}$ is the graph on $n$ vertices with exactly $t$ vertices of degree $n-1$ and the remaining of the $n-t$ vertices forming an independent set. Thus

$$\mathrm{irr}(G) \leq m\sqrt{\frac{2n\left[2m + (n-1)(\Delta - \delta)\right]}{n + \Delta - \delta} - 4m}$$

with equality if and only if $G$ is a regular graph, or $G \cong K_{1,n-1}$.

(iii) Let $G$ be a graph with $n$ vertices, $m$ edges, maximum degree $\Delta$ and minimum degree $\delta$. Then [4]

$$Z(G) \leq 2m(\Delta + \delta) - n\Delta\delta$$

with equality if and only if $G$ has only two types of degrees $\Delta$ and $\delta$. Thus

$$\mathrm{irr}(G) \leq \sqrt{m\left[2mn(\Delta + \delta) - n^2\Delta\delta - 4m^2\right]}$$

with equality if and only if $G$ is a regular graph or $G \cong K_{\Delta,\delta}$.

(iv) Let $G$ be a graph with $n$ vertices, $m$ edges and let $\rho$ be the largest eigenvalue of the adjacency matrix of $G$. Then [9, 12]

$$Z(G) \leq n\rho^2$$

with equality if and only if every component of $G$ is either a regular graph or a semiregular bipartite graph for which the product of two adjacent vertices is equal to $\rho^2$. Thus

$$\mathrm{irr}(G) \leq \sqrt{m\left[n^2\rho^2 - 4m^2\right]}$$

with equality if and only if $G$ is a regular graph or a complete bipartite graph.

# 3 Irregularity of $K_{r+1}$-Free Graphs

In this section we consider the irregularity of $K_{r+1}$-free graphs with $r \geq 2$. We need the following lemma, which was reported in [13]. It may be proved by combining the upper bound for $\rho$ obtained by Nikiforov [11] and the upper bound for $Z(G)$ using $\rho$ in the previous section. However, we reproduce a direct proof [13] here.

**Lemma 1** *Let $G$ be a $K_{r+1}$-free graph with $n$ vertices and $m \geq 1$ edges, where $2 \leq r \leq n-1$. Then*

$$Z(G) \leq \frac{2r-2}{r} nm \tag{1}$$

*with equality if and only if $G$ is a complete bipartite graph for $r = 2$ and a regular complete $r$-partite graph for $r \geq 3$.*

**Proof.** For any $u \in V(G)$, let $c_u$ be the number of edges of the subgraph $G_u$ induced by $N_G(u)$. Since $G_u$ is $K_r$-free, we have by Turán's theorem (see [1]) that $c_u \leq \frac{r-2}{2r-2} d_u^2$ with equality if and only if $G_u$ is a regular complete $(r-1)$-partite graph. It follows that

$$\sum_{v \in N_G(u)} d_v \leq m + c_u \leq m + \frac{r-2}{2r-2} d_u^2$$

and thus

$$Z(G) \leq \sum_{u \in V(G)} \left( m + \frac{r-2}{2r-2} d_u^2 \right) = nm + \frac{r-2}{2r-2} Z(G),$$

from which (1) follows. Suppose that equality holds in (1). Then for any $u \in V(G)$, $G_u$ is a regular complete $(r-1)$-partite graph, and the subgraph induced by $V(G) \setminus N_G(u)$ is an empty graph. Let $v \neq u$ be a vertex that is not adjacent to $u$. Then $d_v < n-1$. If $N_G(v) \neq N_G(u)$, then one of the subgraph induced by $V(G) \setminus N_G(u)$ or $V(G) \setminus N_G(v)$ would not be empty, a contradiction. Thus $G$ is a complete multipartite graph $K_{d_u, \frac{d_u}{r-1}, \ldots, \frac{d_u}{r-1}}$ for any $u \in V(G)$. Now the result follows easily. □

By this lemma and Theorem 1, we have

**Theorem 2** *Let $G$ be a $K_{r+1}$-free graph with $n$ vertices and $m \geq 1$ edges, where $2 \leq r \leq n-1$. Then*

$$irr(G) \leq m \sqrt{\frac{2r-2}{r} n^2 - 4m}$$

*with equality if and only if $G$ is a complete bipartite graph for $r = 2$ and a regular complete $r$-partite graph for $r \geq 3$.*

**Theorem 3** *Let $G$ be a $K_{r+1}$-free graph with $n$ vertices, where $2 \le r \le n-1$. Then*

$$irr(G) < \frac{(r-1)\sqrt{2(r-1)}}{3r\sqrt{3r}}n^3.$$

**Proof.** Let $m$ be the number of edges of $G$. Then [1] $m$ is less than or equal to $\frac{r-1}{2r}n^2$. Note that for $0 \le x \le \frac{r-1}{2r}n^2$ the function

$$f(x) = x\sqrt{\frac{2r-2}{r}n^2 - 4x}$$

decreases if and only if $x \ge \frac{r-1}{3r}n^2$ and that the number of edges of a complete bipartite graph $K_{k,n-k}$ is equal to $k(n-k)$, which is not equal to $\frac{n^2}{6}$, and for $r \ge 3$, the number of edges of a regular complete $r$-partite graph is equal to $\frac{r-1}{2r}n^2$, which is not equal to $\frac{r-1}{3r}n^2$. By Theorem 2,

$$\text{irr}(G) \le f(m) < f\left(\frac{r-1}{3r}n^2\right)$$

from which the result follows. □

**Remark.** Let $G$ be a graph with $n$ vertices. It was shown in [2] that $\text{irr}(G) < \frac{n^3}{9}$ if $G$ is triangle-free, and $\text{irr}(G) \le \frac{n^3}{6\sqrt{3}}$ if $G$ is bipartite. By Theorem 3, $\text{irr}(G) < \frac{n^3}{6\sqrt{3}}$ if $G$ is triangle-free. This improves the above results in [2].

# 4 Irregularity of Trees and Unicyclic Graphs

Let $G$ be a connected graph. Let $V_1(G) = \{v \in V(G) : d_v \ge 3\}$. A pendant vertex is a vertex of degree one.

A connected graph with $n$ vertices and $n-1$ (resp. $n$) edges is known as a tree (resp. unicyclic graph). We now present the maximum possible irregularity of trees and unicyclic graphs of given number of pendant vertices, and characterize the extremal graphs.

Let $V_0(G)$ be the set consisting of one vertex of maximum degree if $G$ is a tree and the set of vertices of the unique cycle of $G$ if $G$ is a unicyclic graph.

**Lemma 2** *Let $G$ be a tree (resp. unicyclic graph) with $n$ vertices and $p \ge 1$ pendant vertices. If $|V_1(G)\backslash V_0(G)| \ge 1$, then there is a tree (resp. unicyclic graph) $G^*$ with $n$ vertices and $p$ pendant vertices such that $d_{G^*}(v) \le 2$ for all $v \in V(G)\backslash V_0(G)$ and $irr(G^*) > irr(G)$.*

**Proof.** Let $x$ be a vertex in $V_0(G)$ whose degree is maximum. Since $|V_1(G)\backslash V_0(G)| \ge 1$, there is a vertex $y$ whose degree is maximum among vertices outside $V_0(G)$.

Then $d_y$ is at least 3. Let $N_G(y) = \{w_1, w_2, \ldots, w_t\}$, where $t = d_y$, $w_1$ lies on the shortest path between $x$ and $y$. Note that $|d_{w_i} - 2| - |d_y - d_{w_i}| \geq -(d_y - 2)$ for $i = 1, 2$. Set $G' = G - \{yw_3, \ldots, yw_t\} + \{xw_3, \ldots, xw_t\}$. Then $G'$ is a tree (resp. unicyclic graph) with $n$ vertices and $p$ pendant vertices.

First suppose that $xy \in E(G)$. Then $x = w_1$. We have

$$\begin{aligned}
& \operatorname{irr}(G') - \operatorname{irr}(G) \\
= & \sum_{i=3}^{t}(|d_x + d_y - 2 - d_{w_i}| - |d_y - d_{w_i}|) \\
& + \sum_{\substack{u \in N_G(x) \\ u \neq y}} (|d_x + d_y - 2 - d_u| - |d_x - d_u|) \\
& + (|d_x + d_y - 2 - 2| - |d_x - d_y|) + (|2 - d_{w_2}| - |d_y - d_{w_2}|) \\
= & (d_x - 2)(d_y - 2) + \sum_{\substack{u \in N_G(x) \\ u \neq y}} (d_x + d_y - 2 - d_u - |d_x - d_u|) \\
& + (d_x + d_y - 4 - |d_x - d_y|) + (|2 - d_{w_2}| - |d_y - d_{w_2}|) \\
\geq & (d_x - 2)(d_y - 2) + \sum_{\substack{u \in N_G(x) \\ u \neq y}} (d_x + d_y - 2 - d_u - |d_x - d_u|) \\
& + (d_x + d_y - 4 - |d_x - d_y|) - (d_y - 2).
\end{aligned}$$

If $d_x \geq d_y$, then $d_x \geq d_u$ for $u \in N_G(x)$ and so

$$\begin{aligned}
& \operatorname{irr}(G') - \operatorname{irr}(G) \\
\geq & (d_x - 2)(d_y - 2) + (d_x - 1)(d_y - 2) + 2d_y - 4 - (d_y - 2) \\
= & 2(d_x - 1)(d_y - 2) > 0.
\end{aligned}$$

Now suppose that $xy \in E(G)$ and $d_x < d_y$ (and then $G$ is a unicyclic graph) or $xy \notin E(G)$. For any neighbor $u$ of $x$ when $G$ is a tree, and for any neighbor $u$ of $x$ in the unique cycle when $G$ is a unicyclic graph, $d_x + d_y - 2 - d_u - |d_x - d_u| = d_y - 2 \geq 1$. For any other neighbor $u$ of $x$ outside $V_0(G)$ when $G$ is a unicyclic graph, since $d_x \geq 3$, we have $d_x + d_y - 2 - d_u - |d_x - d_u| = \min\{d_y - 2, 2d_x + d_y - 2 - 2d_u\} \geq -(d_y - 4)$. If $xy \in E(G)$ and $d_x < d_y$, then

$$\begin{aligned}
& \operatorname{irr}(G') - \operatorname{irr}(G) \\
\geq & (d_x - 2)(d_y - 2) + [2(d_y - 2) - (d_x - 3)(d_y - 4)] \\
& + 2(d_x - 2) - (d_y - 2) \\
= & 2(2d_x + d_y - 7) > 0.
\end{aligned}$$

If $xy \notin E(G)$, then

$$\operatorname{irr}(G') - \operatorname{irr}(G)$$

$$
\begin{aligned}
&= \sum_{i=3}^{t}(|d_x + d_y - 2 - d_{w_i}| - |d_y - d_{w_i}|) \\
&\quad + \sum_{u \in N_G(x)} (|d_x + d_y - 2 - d_u| - |d_x - d_u|) \\
&\quad + \sum_{i=1}^{2}(|d_{w_i} - 2| - |d_y - d_{w_i}|) \\
&\geq (d_x - 2)(d_y - 2) + [2(d_y - 2) - (d_x - 2)(d_y - 4)] - 2(d_y - 2) \\
&= 2(d_x - 2) > 0.
\end{aligned}
$$

Now have proved that $\mathrm{irr}(G^*) > \mathrm{irr}(G)$. Iterating the transformation from $G$ to $G'$ yields the graph $G^*$ as required. □

Let $\mathcal{T}_{n,p}$ be the class of trees with $n$ vertices, $p$ of which are pendant vertices, where $2 \leq p \leq n - 1$. Obviously, if $G \in \mathcal{T}_{n,2}$ then $G \cong P_n$, the path with $n$ vertices, and if $G \in \mathcal{T}_{n,n-1}$ then $G \cong K_{1,n-1}$, the star with $n$ vertices. Let $\mathcal{T}^*_{n,p}$ be the class of trees on $n$ vertices formed by attaching $p$ disjoint paths to a common vertex $v_0$.

**Theorem 4** *Let $G \in \mathcal{T}_{n,p}$. Then*

$$irr(G) \leq p(p-1)$$

*with equality if and only if $G \in \mathcal{T}^*_{n,p}$.*

**Proof.** The cases $p = 2$ and $p = n - 1$ are trivial. Suppose that $3 \leq p \leq n - 2$. If $|V_1(G)| \geq 2$, then by Lemma 2, we have $\mathrm{irr}(G) < \mathrm{irr}(G^*)$ where $T^*$ is a tree in $\mathcal{T}^*_{n,p}$. If $|V_1(G)| = 1$, then $G \in \mathcal{T}^*_{n,p}$ and so

$$\mathrm{irr}(G) = \sum_{i=1}^{p}(d_{v_0} - 1) = \sum_{i=1}^{p}(p-1) = p(p-1).$$

This proves the theorem. □

Finally, we consider unicyclic graphs. Let $\mathcal{U}_{n,p}$ be the class of unicyclic graphs with $n$ vertices, $p$ of which are pendant vertices, where $0 \leq p \leq n - 3$. Obviously, if $G \in \mathcal{U}_{n,0}$ then $G \cong C_n$, the cycle with $n$ vertices. Let $\mathcal{U}^*_{n,p}$ be the class of graphs on $n$ vertices formed by attaching $p$ disjoint paths to a common vertex on a cycle.

**Lemma 3** *Let $G \in \mathcal{U}_{n,p}$ with $C$ being the unique cycle of $G$. If $|V_1(G)| = |V_1(G) \cap V(C)| \geq 2$, then there is a graph $G^* \in \mathcal{U}^*_{n,p}$ such that $irr(G^*) > irr(G)$.*

**Proof.** Since $|V_1(G)| = |V_1(G) \cap V(C)| \geq 2$, there are vertices $x, y \in V_1(C)$ such that $d_x \geq d_y \geq d_v$ for any $v \in V(G)$. Let $N_G(y) = \{w_1, w_2, \ldots, w_t\}$, where $t = d_y$, and $w_1$ and $w_2$ lie on the cycle $C$ and the distance between $x$ and $w_1$ is less than or equal to the distance between $x$ and $w_2$. Note that $d_{w_2} - 2 - |d_y - d_{w_2}| \geq -(d_y - 2)$. Set $G' = G - \{yw_3, \ldots, yw_t\} + \{xw_3, \ldots, xw_t\}$. Then $G' \in \mathcal{U}_{n,p}$.

Suppose that $xy \in E(G)$. Then $x = w_1$. By similar arguments as in the proof of Lemma 2,

$$\begin{aligned}
& \operatorname{irr}(G') - \operatorname{irr}(G) \\
= & \sum_{i=3}^{t} (|d_x + d_y - 2 - d_{w_i}| - |d_y - d_{w_i}|) \\
& + \sum_{\substack{u \in N_G(x) \\ u \neq y}} (|d_x + d_y - 2 - d_u| - |d_x - d_u|) \\
& + (|d_x + d_y - 2 - 2| - |d_x - d_y|) + (|d_{w_2} - 2| - |d_y - d_{w_2}|) \\
= & (d_x - 2)(d_y - 2) + (d_x - 1)(d_y - 2) + 2d_y - 4 + d_{w_2} - 2 - |d_y - d_{w_2}| \\
\geq & (d_x - 2)(d_y - 2) + (d_x - 1)(d_y - 2) + 2d_y - 4 - (d_y - 2) \\
= & 2(d_x - 1)(d_y - 2) > 0.
\end{aligned}$$

Now suppose that $xy \notin E(G)$. We have

$$\begin{aligned}
& \operatorname{irr}(G') - \operatorname{irr}(G) \\
= & \sum_{i=3}^{t} (|d_x + d_y - 2 - d_{w_i}| - |d_y - d_{w_i}|) \\
& + \sum_{u \in N_G(x)} (|d_x + d_y - 2 - d_u| - |d_x - d_u|) \\
& + \sum_{i=1}^{2} (|d_{w_i} - 2| - |d_y - d_{w_i}|) \\
\geq & (d_x - 2)(d_y - 2) + d_x(d_y - 2) - 2(d_y - 2) \\
= & 2(d_x - 2)(d_y - 2) > 0.
\end{aligned}$$

Hence, we have proved that $\operatorname{irr}(G') > \operatorname{irr}(G)$. Iterating the transformation from $G$ to $G'$ yields the graph $G^*$ as required. □

**Theorem 5** *Let $G \in \mathcal{U}_{n,p}$. Then*

$$irr(G) \leq p(p+3)$$

*with equality holds if and only if $G \in \mathcal{U}^*_{n,p}$.*

**Proof.** The case $p = 0$ is trivial. Suppose that $p \geq 1$. Let $C$ be the unique cycle in $G$.

If $|V_1(G) \backslash V(C)| \geq 1$, then by Lemma 2, there is a graph $G^* \in \mathcal{U}_{n,p}$ with $d_{G^*}(v) \leq 2$ for all $v \in V(G) \backslash V(C)$ such that $\mathrm{irr}(G^*) > \mathrm{irr}(G)$.

If $|V_1(G)| = |V_1(G) \cap V(C)| \geq 2$, then by Lemma 3, there is a graph $G^* \in \mathcal{U}^*_{n,p}$ such that $\mathrm{irr}(G^*) > \mathrm{irr}(G)$.

If $|V_1(G)| = |V_1(G) \cap V(C)| = 1$, then $G \in \mathcal{U}^*_{n,p}$ and so

$$\begin{aligned} \mathrm{irr}(G) &= \sum_{i=1}^{p} (d_{v_0} - 1) + 2(d_{v_0} - 2) \\ &= \sum_{i=1}^{p} (p + 2 - 1) + 2(p + 2 - 2) = p(p + 3). \end{aligned}$$

This proves the theorem. □

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