

Remark on the Irregularity of Graphs

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Abstract: Let $G = (V, E)$, $V = \{v_1, v_2, \dots, v_n\}$, $E = \{e_1, e_2, \dots, e_m\}$, be a simple connected graph with the vertex degree sequence $\Delta = d_1 \geq d_2 \geq \dots \geq d_n = \delta > 0$, $d_i = d(v_i)$. The zeroth-order general Randić index, ${}^0R_\alpha(G)$, of a connected graph G , is defined as ${}^0R_\alpha(G) = \sum_{i=1}^n d_i^\alpha$. A linear combination of ${}^0R_\alpha(G)$ of the form $irr^{(\alpha)}(G) = {}^0R_{\alpha+1}(G) - \frac{2m}{n} {}^0R_\alpha(G)$, $\alpha \geq 0$, can be considered as an irregularity measure of a graph since $irr^{(\alpha)}(G) = 0$ if and only if G is a regular graph, and $irr^{(\alpha)}(G) > 0$ otherwise. In this paper we consider a linear combination $irr^{(\alpha)}(G) - \frac{2m}{n} irr^{(\alpha-1)}(G)$, for $\alpha \geq 1$, which can be also considered as irregularity measure of graph, and determine its bounds.

Keywords: Topological indices, irregularity (of a graph).

1 Introduction

Let $G = (V, E)$, $V = \{v_1, v_2, \dots, v_n\}$, $E = \{e_1, e_2, \dots, e_m\}$, be a simple connected graph with the vertex degree sequence $\Delta = d_1 \geq d_2 \geq \dots \geq d_n = \delta > 0$, $d_i = d(v_i)$.

A topological index, or graph invariant, for a graph is a numerical quantity which is invariant under isomorphism of the graph. The study of the mathematical aspects of the degree-based graph invariants (also known as topological indices) is considered to be one of the very active research areas within the field of chemical graph theory.

The first Zagreb index [1] is a vertex-degree based graph invariant defined as [2]

$$M_1(G) = \sum_{i=1}^n d_i^2.$$

The first Zagreb index is the oldest and most extensively studied graph-based molecular structure descriptor. Details about its applications and mathematical properties can be found in surveys [3–7] and in the references cited therein.

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Various generalizations of the first Zagreb index have been proposed. In [8] a so called zeroth-order general Randić index was introduced. It is defined as

$${}^0R_\alpha(G) = \sum_{i=1}^n d_i^\alpha,$$

where α is an arbitrary real number. This index is also met in the literature under the names first general Zagreb index [9], or variable first Zagreb index [10]. For some particular values of α the following indices/values are obtained

- The modified first Zagreb index [7] is obtained for $\alpha = -2$, that is ${}^mM_1(G) = {}^0R_{-2}(G)$;
- The inverse degree index [11] is obtained for $\alpha = -1$, that is $ID(G) = {}^0R_{-1}(G)$;
- For $\alpha = 0$ we have ${}^0R_0(G) = n$;
- For $\alpha = 1$, we have ${}^0R_1(G) = \sum_{i=1}^n d_i = 2m$;
- The first Zagreb index is obtained for $\alpha = 2$, $M_1(G) = {}^0R_2(G)$
- The forgotten topological index [12] is obtained for $\alpha = 3$, $F(G) = {}^0R_3(G)$.

A graph G is called regular if all its vertices have the same degree. Any mapping that associates a real number $IM(G)$ to a graph G , satisfying the condition $IM(G) = 0$ if and only if G is regular, and $IM(G) > 0$ otherwise, can be used as an irregularity measure. On various irregularity measures the reader can refer to [13–21].

2 Preliminaries

In [14] it was proven that for any real $\alpha \geq 0$ holds

$${}^0R_{\alpha+1}(G) \geq \frac{2m}{n} {}^0R_\alpha(G), \quad (2.1)$$

with equality if and only if $\alpha = 0$, or G is regular. When $\alpha < 0$ the sense of inequality (2.1) reverses, that is

$${}^0R_\alpha(G) \geq \frac{n}{2m} {}^0R_{\alpha+1}(G). \quad (2.2)$$

From the inequality (2.1) for $\alpha > 0$, a number of irregularity measures can be derived:

$$irr^{(\alpha)}(G) = {}^0R_{\alpha+1}(G) - \frac{2m}{n} {}^0R_\alpha(G). \quad (2.3)$$

Thus, for $\alpha = 1$, we obtain the well known Edwards irregularity measure [13, 20, 23]:

$$irr^{(1)}(G) = M_1(G) - \frac{4m^2}{n}. \quad (2.4)$$

This irregularity measure is closely related to the irregularity measure introduced by Bell [14], and defined as

$$irr_B(G) = \frac{1}{n} \sum_{i=1}^n \left(d_i - \frac{2m}{n} \right)^2.$$

Namely, the following is valid [13]:

$$irr^{(1)}(G) = n \cdot irr_B(G).$$

In [14] the following inequality was proven

$$\frac{1}{2}(\Delta - \delta)^2 \leq irr^{(1)}(G) \leq n\alpha(n)(\Delta - \delta)^2, \quad (2.5)$$

where

$$\alpha(n) = \frac{1}{4} \left(1 - \frac{1 + (-1)^{n+1}}{2n^2} \right).$$

From the inequality (2.2) for $\alpha < 0$, one can derive the following family of irregularity measures

$$irr^{(\alpha)}(G) = {}^0R_\alpha(G) - \frac{n}{2m} {}^0R_{\alpha+1}(G). \quad (2.6)$$

Here we are interested for the irregularity measure obtained from (2.6) for the case $\alpha = -1$, that is

$$irr^{(-1)}(G) = ID(G) - \frac{n^2}{2m}. \quad (2.7)$$

In [25] the following inequalities were proven

$$\frac{1}{\Delta + \delta} \left(\sqrt{\frac{\Delta}{\delta}} - \sqrt{\frac{\delta}{\Delta}} \right)^2 \leq irr^{(-1)}(G) \leq \frac{n(n-1)}{4m} \left(\sqrt{\frac{\Delta}{\delta}} - \sqrt{\frac{\delta}{\Delta}} \right)^2. \quad (2.8)$$

In [26] it was proven that for any real $\alpha \geq 0$ holds

$${}^0R_{\alpha+1}(G) \geq \frac{(2m)^{\alpha+1}}{n^\alpha}. \quad (2.9)$$

It is not difficult to observe that the above inequality also holds when $\alpha \leq -1$, and that when $-1 \leq \alpha \leq 0$ the opposite inequality is valid. Equality in (2.9) holds if and only if either $\alpha = -1$, or $\alpha = 0$, or G is a regular graph.

For $\alpha \leq -1$ or $\alpha \geq 0$, from the inequality (2.9) one can derive a family of irregularity measures of the form

$$irr_\alpha(G) = {}^0R_{\alpha+1}(G) - \frac{(2m)^{\alpha+1}}{n^\alpha}. \quad (2.10)$$

It is not difficult to observe that for $\alpha = 1$ (2.10) coincides with (2.4), and for $\alpha = -2$ it coincides with (2.7), that is that the following is valid

$$irr^{(1)}(G) = irr_1(G) \quad \text{and} \quad irr^{(-1)}(G) = irr_{-2}(G).$$

Particularly interesting for us are irregularity measures obtained from (2.10) for $\alpha = -3$ and $\alpha = 2$, that is

$$\text{irr}_{-3}(G) = {}^m M_1(G) - \frac{n^3}{4m^2} \quad \text{and} \quad \text{irr}_2(G) = F(G) - \frac{8m^3}{n^2}. \quad (2.11)$$

In this paper we consider bounds of the expression

$$\text{irr}^{(\alpha)}(G) - \frac{2m}{n} \text{irr}^{(\alpha-1)}(G), \quad (2.12)$$

where α is an arbitrary real number. When $\alpha \geq 1$ the expression (2.12) can be considered as an irregularity measure. New bounds for topological indices $M_1(G)$ and $F(G)$ are obtained as special cases.

3 Main results

First we recall one inequality for real number sequences that will be frequently used later in this paper.

Lemma 3.1. [27] *Let $p = (p_i)$, $i = 1, 2, \dots, n$, be a sequence of non negative real numbers and $a = (a_i)$, $i = 1, 2, \dots, n$, a sequence of positive real numbers. Then, for any real r , $r \leq 0$ or $r \geq 1$, we have that*

$$\left(\sum_{i=1}^n p_i \right)^{r-1} \sum_{i=1}^n p_i a_i^r \geq \left(\sum_{i=1}^n p_i a_i \right)^r. \quad (3.1)$$

When $0 \leq r \leq 1$, the opposite inequality is valid. Equality holds if and only if either $r = 0$, or $r = 1$, or $a_1 = a_2 = \dots = a_n$, or $p_1 = \dots = p_t = 0$ and $a_{t+1} = \dots = a_n$, or $a_1 = \dots = a_t$ and $p_{t+1} = \dots = p_n = 0$, for some t , $1 \leq t \leq n-1$.

More on the above inequality can be found in [28, 29].

Theorem 3.1. *Let G be a connected irregular graph with $n \geq 3$ vertices and m edges. Then, for any real α , $\alpha \leq 0$ or $\alpha \geq 1$, we have that*

$$\text{irr}^{(\alpha-1)}(G) - \frac{2m}{n} \text{irr}^{(\alpha-2)}(G) \geq \frac{4 \left(\frac{m}{n}\right)^{\alpha+1} \text{irr}_{-2}(G)^\alpha}{\left(\frac{m}{n} \text{irr}_{-3}(G) - \text{irr}_{-2}(G)\right)^{\alpha-1}}. \quad (3.2)$$

When $0 \leq \alpha \leq 1$ the opposite inequality is valid. Equality holds if and only if $\alpha = 0$ or $\alpha = 1$.

Proof. For $r = \alpha$, $\alpha \leq 0$ or $\alpha \geq 1$, $p_i = \frac{(d_i - \frac{2m}{n})^2}{d_i^2}$, $a_i = d_i$, $i = 1, 2, \dots, n$, the inequality (3.1) becomes

$$\left(\sum_{i=1}^n \frac{(d_i - \frac{2m}{n})^2}{d_i^2} \right)^{\alpha-1} \sum_{i=1}^n \left(d_i - \frac{2m}{n} \right)^2 d_i^{\alpha-2} \geq \left(\sum_{i=1}^n \frac{(d_i - \frac{2m}{n})^2}{d_i} \right)^\alpha. \quad (3.3)$$

On the other hand, the following identities are valid

$$\begin{aligned}
\sum_{i=1}^n \frac{(d_i - \frac{2m}{n})^2}{d_i^2} &= \sum_{i=1}^n \left(1 - \frac{4m}{n} \frac{1}{d_i} + \frac{4m^2}{n^2} \frac{1}{d_i^2} \right) = \\
&= n - \frac{4m}{n} ID(G) + \frac{4m^2}{n^2} {}^m M_1(G) = \\
&= 2n - \frac{4m}{n} ID(G) + \frac{4m^2}{n^2} {}^m M_1(G) - n = \\
&= \frac{4m^2}{n^2} \left({}^m M_1(G) - \frac{n^3}{4m^2} \right) - \frac{4m}{n} \left(ID(G) - \frac{n^2}{2m} \right).
\end{aligned}$$

From the above identity and inequalities (2.7) and (2.11), we obtain

$$\sum_{i=1}^n \frac{(d_i - \frac{2m}{n})^2}{d_i^2} = \frac{4m}{n} \left(\frac{m}{n} irr_{-3}(G) - irr_{-2}(G) \right). \quad (3.4)$$

Since

$$\begin{aligned}
\sum_{i=1}^n \left(d_i - \frac{2m}{n} \right)^2 d_i^{\alpha-2} &= \sum_{i=1}^n \left(d_i^\alpha - \frac{4m}{n} d_i^{\alpha-1} + \frac{4m^2}{n^2} d_i^{\alpha-2} \right) = \\
&= {}^0 R_\alpha(G) - \frac{4m}{n} {}^0 R_{\alpha-1}(G) + \frac{4m^2}{n^2} {}^0 R_{\alpha-2}(G) = \\
&= {}^0 R_\alpha(G) - \frac{2m}{n} {}^0 R_{\alpha-1}(G) - \frac{2m}{n} \left({}^0 R_{\alpha-1}(G) - \frac{2m}{n} {}^0 R_{\alpha-2}(G) \right) = \\
&= irr^{(\alpha-1)}(G) - \frac{2m}{n} irr^{(\alpha-2)}(G),
\end{aligned} \quad (3.5)$$

and

$$\begin{aligned}
\sum_{i=1}^n \frac{(d_i - \frac{2m}{n})^2}{d_i} &= \sum_{i=1}^n \left(d_i - \frac{4m}{n} + \frac{4m^2}{n^2} \frac{1}{d_i} \right) = \\
&= 2m - 4m + \frac{4m^2}{n^2} ID(G) = \frac{4m^2}{n^2} \left(ID(G) - \frac{n^2}{2m} \right) = \frac{4m^2}{n^2} irr_{-2}(G),
\end{aligned} \quad (3.6)$$

from identities (3.4), (3.5), (3.6) and inequality (3.3) we obtain

$$\begin{aligned}
\left(\frac{4m}{n} \right)^{\alpha-1} \left(\frac{m}{n} irr_{-3}(G) - irr_{-2}(G) \right)^{\alpha-1} \left(irr^{(\alpha-1)}(G) - \frac{2m}{n} irr^{(\alpha-2)}(G) \right) &\geq \\
&\geq \left(\frac{4m^2}{n^2} \right)^\alpha irr_{-2}(G)^\alpha.
\end{aligned}$$

Since G is irregular, we have that $irr_{-2}(G) > 0$ and $\frac{m}{n} irr_{-3}(G) - irr_{-2}(G) > 0$, from the above inequality follows (3.2).

The case when $0 \leq \alpha \leq 1$ can be proved similarly. Since G is irregular, equality in (3.3), and consequently in (3.2), holds if and only if $\alpha = 0$ or $\alpha = 1$. \square

Corollary 3.1. *Let G be a connected irregular graph with $n \geq 3$ vertices and m edges. Then we have*

$$M_1(G) \geq \frac{4m^2}{n} + \frac{4\left(\frac{m}{n}\right)^3 \text{irr}_{-2}(G)^2}{\frac{m}{n} \text{irr}_{-3}(G) - \text{irr}_{-2}(G)}. \quad (3.7)$$

Proof. For $\alpha = 2$ the inequality (3.2) becomes

$$\text{irr}^{(1)}(G) - \frac{2m}{n} \text{irr}^{(0)}(G) \geq \frac{4\left(\frac{m}{n}\right)^3 \text{irr}_{-2}(G)^2}{\frac{m}{n} \text{irr}_{-3}(G) - \text{irr}_{-2}(G)}. \quad (3.8)$$

Since

$$\text{irr}^{(0)}(G) = {}^0R_1(G) - \frac{2m}{n} {}^0R_0(G) = 2m - 2m = 0,$$

and having in mind identity (2.4) and inequality (3.8), we arrive at (3.7). \square

Remark 3.1. *The inequality (3.7) is stronger than*

$$M_1(G) \geq \frac{4m^2}{n} + \frac{4\left(\frac{m}{n}\right)^2 \text{irr}_{-2}(G)^2}{\text{irr}_{-3}(G)},$$

which was proven in [30].

Corollary 3.2. *Let G be a connected irregular graph with $n \geq 3$ vertices and m edges. Then we have*

$$F(G) \geq \frac{4m}{n} M_1(G) - \frac{8m^3}{n^2} + \frac{4\left(\frac{m}{n}\right)^4 \text{irr}_{-2}(G)^3}{\left(\frac{m}{n} \text{irr}_{-3}(G) - \text{irr}_{-2}(G)\right)^2}.$$

Corollary 3.3. *Let G be a connected graph with $n \geq 2$ vertices and m edges. Then*

$$F(G) - \frac{8m^3}{n^2} \geq \frac{4m}{n} \left(M_1(G) - \frac{4m^2}{n} \right),$$

$$F(G) \geq \frac{2m}{n} M_1(G), \quad (3.9)$$

$$F(G) \geq \frac{8m^3}{n^2}. \quad (3.10)$$

Equalities hold if and only if G is regular.

Remark 3.2. *The inequality (3.9) was proven in [31], whereas (3.10) in [9] (see also [26]).*

Corollary 3.4. *Let U , $U \not\cong C_n$, be a connected unicyclic graph with $n \geq 4$ vertices. Then*

$$M_1(U) \geq 4n + \frac{4 \text{irr}_{-2}(U)^2}{\text{irr}_{-3}(U) - \text{irr}_{-2}(U)}, \quad (3.11)$$

and

$$F(U) \geq 4M_1(U) - 8n + \frac{4 \text{irr}_{-2}(U)^3}{\left(\text{irr}_{-3}(U) - \text{irr}_{-2}(U)\right)^2}. \quad (3.12)$$

Remark 3.3. When U , $U \not\cong C_n$, is connected unicyclic graph with $n \geq 4$, the inequality (3.11) is stronger than

$$M_1(U) \geq 4n,$$

which was proven in [32], whereas the inequality (3.12) is stronger than

$$F(U) \geq 4M_1(U) - 8n.$$

The proof of the next theorem is analogous to that of Theorem 3.1, hence omitted.

Theorem 3.2. Let G be a connected irregular graph with $n \geq 3$ vertices and m edges. Then, for any real α , $\alpha \leq 0$ or $\alpha \geq 1$, we have that

$$\text{irr}^{(\alpha)}(G) - \frac{2m}{n} \text{irr}^{(\alpha-1)}(G) \geq \frac{n^{2\alpha-2} \text{irr}_1(G)^\alpha}{(2m)^{2\alpha-2} \text{irr}_{-2}(G)^{\alpha-1}}. \quad (3.13)$$

When $0 \leq \alpha \leq 1$, the opposite inequality is valid. Equality holds if and only if $\alpha = 0$ or $\alpha = 1$.

Corollary 3.5. Let G be a connected graph with $n \geq 2$ vertices and m edges. Then for any real $\alpha > 1$, holds

$$\text{irr}^{(\alpha)}(G) - \frac{2m}{n} \text{irr}^{(\alpha-1)}(G) \geq \frac{n^{\alpha-1} (\Delta - \delta)^2 (\Delta \delta)^{\alpha-1}}{2^\alpha m^{\alpha-1} (n-1)^{\alpha-1}}.$$

Equality holds if and only if G is regular.

Proof. The required result immediately follows from (3.13), left-hand side of (2.5) and right-hand side of (2.8). \square

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