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INVERSE DEGREE INVARIANT OF GRAPHS

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ABSTRACT. Degree based topological invariants are very important to study the properties of molecular graphs. In this paper, some results related to inverse degree invariant are obtained.

1. INTRODUCTION

For a vertex $z \in V(\mathcal{T})$, the valency of the vertex z in $\mathcal{T}$, denoted by $\beta_{\mathcal{T}}(z)$, is the number of edges incident to z in $\mathcal{T}$. A topological invariant of a graph is a number related to the graph; it does not depend on labeling of the graph. Several types of such invariants exist, especially those based on distance and degree. One of the most important discussed topological invariant is the Wiener invariant. The first degree based invariants defined by Gutman et al. in 1982 which are related to QSPR and QSAR studies.

- First Zagreb Invariant: $M_1(\mathcal{T}) = \sum_{z\in V(\mathcal{T})} \beta^2_{\mathcal{T}}(z) = \sum_{a_1a_2\in E(\mathcal{T})} (\beta_{\mathcal{T}}(a_1)+\beta_{\mathcal{T}}(a_2))$.
- Second Zagreb Invariant: $M_2(\mathcal{T}) = \sum_{a_1a_2\in E(\mathcal{T})} \beta_{\mathcal{T}}(a_1)\beta_{\mathcal{T}}(a_2)$.
- F-invariant: $F(\mathcal{T}) = \sum_{z\in V(\mathcal{T})} \beta^3_{\mathcal{T}}(z)$.
- Harmonic invariant: $\sum_{a_1a_2\in E(\mathcal{T}_1)} \frac{2}{\beta_{\mathcal{T}_1}(a_1)+\beta_{\mathcal{T}_1}(a_2)}$.
- Inverse degree invariant: $ID(\mathcal{T}) = \sum_{z\in V(\mathcal{T})} \frac{1}{\beta_{\mathcal{T}}(z)}$.

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The inverse degree invariant attracted attention through conjectures of the computer program Graffiti [2]. It has been viewed by several authors, see [1,3–5]. In this paper, we have obtained the results related to inverse degree invariant of a connected graphs.

2. Main results

In this section, first we obtain the bounds for the inverse degree invariant of a connected graph.

Theorem 2.1. *Let $\mathcal{T}$ be a (s,r)-graph. Then $ID(\mathcal{T}) \geq s\Big(1 - ln\ (\Delta(\mathcal{T}))\Big)$ with equality if and only if $\mathcal{T}$ is a path on two vertices.*

Proof. Assume the function $f(Z) = Z - ln\, Z - 1$. Easy calculation gives $f(Z) \geq 0$. Hence for any vertex x in $V(\mathcal{T})$, $\frac{1}{\beta_{\mathcal{T}}(x)} - ln\ \left(\frac{1}{\beta_{\mathcal{T}}(x)}\right) - 1 \geq 0$. So, $\frac{1}{\beta_{\mathcal{T}}(x)} \geq 1 + ln\ \left(\frac{1}{\beta_{\mathcal{T}}(x)}\right)$. By taking the summation over the vertices of the graph, we get $ID(\mathcal{T}) \geq s + \sum\limits_{x \in V(\mathcal{T})} ln\ \left(\frac{1}{\beta_{\mathcal{T}}(x)}\right) = s + ln\ \left(\prod\limits_{x \in V(\mathcal{T})} \frac{1}{\beta_{\mathcal{T}}(x)}\right) \geq s + ln\ \left(\frac{1}{(\Delta(\mathcal{T}))^s}\right) = s - s\, ln\ (\Delta(\mathcal{T})) = s\Big(1 - ln\ (\Delta(\mathcal{T}))\Big)$.

To show the equality, let $f(Z) = 0$, then $Z = 1$. Thus $\frac{1}{\beta_{\mathcal{T}}(x)} = 1$ for any vertex $x \in V(\mathcal{T})$. Hence $\beta_{\mathcal{T}}(x) = 1$ for every vertex $x \in V(\mathcal{T})$, which holds if and only if $\mathcal{T}$ is a path on two vertices. □

Theorem 2.2. *Let $\mathcal{T}$ be (s,r)-graph. Then $IDD(\mathcal{T}) \geq 2(s-r)$ with equality if and only if $\mathcal{T}$ is a path on two vertices.*

Proof. Assume the function $f(Z) = Z + \frac{1}{Z} - 2$. Easy calculation gives $f(Z) \geq 0$. Hence for any vertex x in $\mathcal{T}$, $\frac{1}{\beta_{\mathcal{T}}(x)} + \beta_{\mathcal{T}}(x) - 2 \geq 0$. By taking the summation over the vertices of the graph, we get $ID(\mathcal{T}) \geq 2s - \sum\limits_{x \in V(\mathcal{T})} \beta_{\mathcal{T}}(x) = 2s - 2t = 2(s-r)$.

To show the equality, let $f(Z) = 0$, then $Z = 1$. Thus $\frac{1}{\beta_{\mathcal{T}}(x)} = 1$ for any vertex $x \in V(\mathcal{T})$. Hence $\beta_{\mathcal{T}}(x) = 1$ for every vertex $x \in V(\mathcal{T})$, which holds if and only if $\mathcal{T}$ is a path on two vertices.

- Subdivision graph $S(\mathcal{T})$ is the graph obtained from $\mathcal{T}$ by replacing each edge of $\mathcal{T}$ by a path of length 2.

- The graph $R(\mathcal{T})$ is obtained from $\mathcal{T}$ by adding a new vertex corresponding to each edge of $\mathcal{T}$, then joining each new vertex to the end vertices of the corresponding edge.
- The join of two graphs $\mathcal{T}_1$ and $\mathcal{T}_2$, denoted by $\mathcal{T}_1 \vee \mathcal{T}_2$, is the union $\mathcal{T}_1 \cup \mathcal{T}_2$ together with all the edges joining $V(\mathcal{T}_1)$ and $V(\mathcal{T}_2)$.
- The vertex S-join graph $\mathcal{T}_1 \vee_S \mathcal{T}_2$ is obtained from $S(\mathcal{T}_1)$ and $\mathcal{T}_2$ by joining each vertex of $V(\mathcal{T}_1)$ to every vertex of $\mathcal{T}_2$.
- The vertex R-join graph $\mathcal{T} \vee_S \mathcal{T}_2$, is obtained from $R(\mathcal{T}_1)$ and $\mathcal{T}_2$ by joining each vertex of $V(\mathcal{T}_1)$ to every vertex of $\mathcal{T}_2$.

□

Lemma 2.1. *Let $\mathcal{T}_1$ and $\mathcal{T}_2$ be two connected graphs with $|V(\mathcal{T}_1)| = s_1$ and $|V(\mathcal{T}_1)| = s_2$. Then*
(i) The valency of a vertex z in $\mathcal{T}_1 \vee_S \mathcal{T}_2$ is

$$\beta_{\mathcal{T}_1 \vee_S \mathcal{T}_2}(z) = \begin{cases} \beta_{\mathcal{T}_1}(z) + s_2, \text{ if } z \in V(\mathcal{T}_1) \\ \beta_{\mathcal{T}_2}(z) + s_1, \text{ if } z \in V(\mathcal{T}_2) \\ 2, \text{ if } z \in I(\mathcal{T}_1). \end{cases}.$$

(ii) The valency of a vertex z in $\mathcal{T}_1 \vee_R \mathcal{T}_2$ is

$$\beta_{\mathcal{T}_1 \vee_R \mathcal{T}_2}(z) = \begin{cases} \beta_{\mathcal{T}_1}(z) + s_2, \text{ if } z \in V(\mathcal{T}_1) \\ \beta_{\mathcal{T}_2}(z) + s_1, \text{ if } z \in V(\mathcal{T}_2) \\ 2, \text{ if } z \in I(\mathcal{T}_1). \end{cases}.$$

Lemma 2.2. *[6] Let g be a convex function on the interval K and $c_1, c_2, \ldots, c_t \in K$. Then $g\left(\frac{c_1+c_2+\ldots+c_t}{t}\right) \leq \frac{g(c_1)+g(c_2)+\ldots g(c_t)}{t}$, with equality if and only if $c_1 = c_2 = \ldots = c_t$.*

Theorem 2.3. *Let G_i be a graph with s_i vertices and t_i edges, $i = 1, 2$. Then*

(i) $ID(\mathcal{T}_1 \vee_S \mathcal{T}_2) \leq \frac{ID(\mathcal{T}_1)+ID(\mathcal{T}_2)}{4} + \frac{s_1^2+s_2^2}{4s_1s_2} + \frac{t_1}{2}$.
(ii) $ID(\mathcal{T}_1 \vee_R \mathcal{T}_2) \leq \frac{ID(\mathcal{T}_1)+2ID(\mathcal{T}_2)}{8} + \frac{s_1^2+s_2^2}{4s_1s_2} + \frac{t_1}{2}$.

Proof. From the definition of inverse degree invariant, we have

$$\begin{aligned} ID(\mathcal{T}_1 \vee_S \mathcal{T}_2) &= \sum_{z\in V(\mathcal{T}_1\vee_S\mathcal{T}_2)} \frac{1}{\beta_{\mathcal{T}_1\vee_S\mathcal{T}_2}(z)} \\ &= \sum_{z\in V(\mathcal{T}_1)} \frac{1}{\beta_{\mathcal{T}_1\vee_S\mathcal{T}_2}(z)} + \sum_{z\in V(\mathcal{T}_2)} \frac{1}{\beta_{\mathcal{T}_1\vee_S\mathcal{T}_2}(z)} + \sum_{z\in I(\mathcal{T}_1)} \frac{1}{\beta_{\mathcal{T}_1\vee_S\mathcal{T}_2}(z)}. \end{aligned}$$

By Lemma 2.1 (i), we get

$$ID(\mathcal{T}_1 \vee_S \mathcal{T}_2) = \sum_{z\in V(\mathcal{T}_1)} \frac{1}{\beta_{\mathcal{T}_1}(z)+s_2} + \sum_{z\in V(\mathcal{T}_2)} \frac{1}{\beta_{\mathcal{T}_2}(z)+s_1} + \sum_{z\in I(\mathcal{T}_1)} \frac{1}{2}.$$

By Jonson's inequality, we obtain

$$ID(\mathcal{T}_1 \vee_S \mathcal{T}_2) \leq \frac{1}{4}\sum_{z\in V(\mathcal{T}_1)} \left(\frac{1}{\beta_{\mathcal{T}_1}(z)} + \frac{1}{s_2}\right) + \frac{1}{4}\sum_{z\in V(\mathcal{T}_2)} \left(\frac{1}{\beta_{\mathcal{T}_2}(z)} + \frac{1}{s_1}\right) + \sum_{z\in I(\mathcal{T}_1)} \frac{1}{2}.$$

From the definition of inverse degree invariant, we have

$$ID(\mathcal{T}_1 \vee_S \mathcal{T}_2) = \frac{ID(\mathcal{T}_1)+ID(\mathcal{T}_2)}{4} + \frac{s_1^2+s_2^2}{4s_1s_2} + \frac{t_1}{2}.$$

From Lemma 2.1 (ii) and similar argument of (i), we get the result of (ii). □

- The graph $Q(\mathcal{T})$ is obtained from the graph $\mathcal{T}$ by inserting a new vertex into each edge of $\mathcal{T}$, then joining with edges those pairs of new vertices on adjacent edges of $\mathcal{T}$.
- The total graph $T(\mathcal{T})$ has as its vertices the edges and vertices of $\mathcal{T}$. Adjacency in $T(\mathcal{T})$ is defined as adjacency or incidence for the corresponding elements of $\mathcal{T}$.
- The vertex Q-join graph $\mathcal{T}_1 \vee_Q \mathcal{T}_2$ is obtained from $Q(\mathcal{T}_1)$ and $\mathcal{T}_2$ by joining each vertex of $V(\mathcal{T}_1)$ to every vertex of $\mathcal{T}_2$.
- The vertex T-join graph $\mathcal{T} \vee_T \mathcal{T}_2$ is obtained from $T(\mathcal{T}_1)$ and $\mathcal{T}_2$ by joining each vertex of $V(\mathcal{T}_1)$ to every vertex of $\mathcal{T}_2$.

Lemma 2.3. *Let $\mathcal{T}_1$ and $\mathcal{T}_2$ be two connected graphs. Then*

(i) *The valency of z in $\mathcal{T}_1 \vee_Q \mathcal{T}_2$ is*

$$\beta_{\mathcal{T}_1\vee_Q\mathcal{T}_2}(z) = \begin{cases} \beta_{\mathcal{T}_1}(z) + |V(\mathcal{T}_2)|\,, & \text{if } z \in V(\mathcal{T}_1) \\ \beta_{\mathcal{T}_2}(z) + |V(\mathcal{T}_1)|\,, & \text{if } z \in V(\mathcal{T}_2) \\ \beta_{\mathcal{T}_1}(x) + \beta_{\mathcal{T}_1}(y), & \text{if } e = xy \in I(\mathcal{T}_1). \end{cases}.$$

(ii) *The valency of z in $\mathcal{T}_1 \vee_T \mathcal{T}_2$ is*

$$\beta_{\mathcal{T}_1 \vee_T \mathcal{T}_2}(z) = \begin{cases} 2d_{\mathcal{T}_1}(z) + |V(\mathcal{T}_2)|\,, \text{ if } z \in V(\mathcal{T}_1) \\ \beta_{\mathcal{T}_2}(z) + |V(\mathcal{T}_1)|\,, \text{ if } z \in V(\mathcal{T}_2) \\ \beta_{\mathcal{T}_1}(x) + \beta_{\mathcal{T}_1}(y), \text{ if } e = xy \in I(\mathcal{T}_1). \end{cases}.$$

Theorem 2.4. *Let G_i be a graph with s_i vertices and t_i edges, $i = 1, 2$. Then*

(i) $ID(\mathcal{T}_1 \vee_Q \mathcal{T}_2) \leq \frac{ID(\mathcal{T}_1)+ID(\mathcal{T}_2)}{4} + \frac{s_1^2+s_2^2}{4s_1s_2} + \frac{H(\mathcal{T}_1)}{2}$.

(ii) $ID(\mathcal{T}_1 \vee_T \mathcal{T}_2) \leq \frac{ID(\mathcal{T}_1)+2ID(\mathcal{T}_2)}{8} + \frac{s_1^2+s_2^2}{4s_1s_2} + \frac{H(\mathcal{T}_1)}{2}$.

Proof. From the definition of inverse degree invariant, we obtain

$$\begin{aligned} ID(\mathcal{T}_1 \vee_Q \mathcal{T}_2) &= \sum_{z \in V(\mathcal{T}_1 \vee_Q \mathcal{T}_2)} \frac{1}{\beta_{\mathcal{T}_1 \vee_Q \mathcal{T}_2}(z)} \\ &= \sum_{z \in V(\mathcal{T}_1)} \frac{1}{\beta_{\mathcal{T}_1 \vee_Q \mathcal{T}_2}(z)} + \sum_{z \in V(\mathcal{T}_2)} \frac{1}{\beta_{\mathcal{T}_1 \vee_Q \mathcal{T}_2}(z)} + \sum_{z \in I(\mathcal{T}_1)} \frac{1}{\beta_{\mathcal{T}_1 \vee_Q \mathcal{T}_2}(z)}. \end{aligned}$$

By Lemma 2.3 (i), we get

$$ID(\mathcal{T}_1 \vee_Q \mathcal{T}_2) = \sum_{z \in V(\mathcal{T}_1)} \frac{1}{\beta_{\mathcal{T}_1}(z) + s_2} + \sum_{z \in V(\mathcal{T}_2)} \frac{1}{\beta_{\mathcal{T}_2}(z) + s_1} + \sum_{z \in I(\mathcal{T}_1)} \frac{1}{\beta_{I(\mathcal{T}_1)}(z)}.$$

By Jenson's inequality, we have

$$\begin{aligned} ID(\mathcal{T}_1 \vee_Q \mathcal{T}_2) &\leq \frac{1}{4} \sum_{z \in V(\mathcal{T}_1)} \left(\frac{1}{\beta_{\mathcal{T}_1}(z)} + \frac{1}{s_2} \right) + \frac{1}{4} \sum_{z \in V(\mathcal{T}_2)} \left(\frac{1}{\beta_{\mathcal{T}_2}(z)} \right. \\ &\quad \left. + \frac{1}{s_1} \right) + \sum_{z_1 z_2 \in E(\mathcal{T}_1)} \frac{1}{\beta_{\mathcal{T}_1}(z_1) + \beta_{\mathcal{T}_1}(z_2)} \\ &= \frac{ID(\mathcal{T}_1) + ID(\mathcal{T}_2)}{4} + \frac{s_1^2 + s_2^2}{4s_1s_2} + \frac{H(\mathcal{T}_1)}{2} \end{aligned}$$

Apply Lemma 2.3 (ii) and a similar argument of (i), we obtain the result of (ii). □

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