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Bounds on Degree Inverse Indices of Graphs

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Abstract:
Topological indices play an important role in representing molecular structures by capturing information related to their chemical properties and possible interactions. These indices are widely applied in Quantitative Structure Activity Relationship (QSAR) studies, where they assist in linking molecular structure with biological activity and other physicochemical characteristics. In this work, explicit expressions for the degree inverse indices of transformation graphs are derived.

Keywords: chemical graph theory, transformation graph, degree-based topological index.
MSC: 05C35, 05C07, 05C40

Introduction

Graph-theoretical concepts are widely applied in chemistry to model molecular systems. When materials are examined at the nanoscale, their properties often differ substantially from those observed at the macroscopic level, which makes numerical analysis a key component of nanoscale studies. Chemical graph theory, an interdisciplinary area of mathematics, utilizes graph-based methods to represent and analyze the structural features of chemical compounds [2, 3]. In mathematical chemistry, topological indices (TIs) provide numerical descriptors of molecular structures and are extensively used to estimate a variety of chemical and biological properties without experimental procedures. These indices encode the structural information of molecules through their corresponding molecular graphs. Based on their defining parameters, TIs are generally categorized as distance-based, degree-based, or eigenvalue-based indices [10–12]. The present work investigates degree-based topological indices associated with transformation graphs. Introduced by Gutman and Trinajstic [4] in 1972, and Das and Gutman [5] the first and second Zagreb indices respectively of the graph G are given by

$$\mathrm{M}_1(\psi) = \sum_{ts\in E(\psi)} \left(\delta(t) + \delta(s)\right)$$

and

$$\mathrm{M}_2(\psi) = \sum_{ts\in E(\psi)} \delta(t)\delta(s).$$

The degree inverse index of Ψ is defined as

$$\mathrm{M}_{\mathrm{DII}}(\psi) = \sum_{t\in V(\psi)} \frac{1}{\delta(t)} = \sum_{ts\in E(\psi)} \left(\frac{1}{\delta(t)^2} + \frac{1}{\delta(s)^2}\right)$$

Other related indices have attracted great interest in the last ten years. Among them we can mention the harmonic degree index [1]. For a graph Ψ, the harmonic degree index $\mathrm{M}_{\mathrm{HDI}}$ is defined as

$$M_{HDI}(\Psi) = \sum_{ts\in E(\psi)} \frac{2}{\delta(t) + \delta(s)}$$

The symmetric deg index of Ψ is defined as

$$M_{S\,D}(\psi) \;=\; \sum_{ts\in E(\psi)} \left(\frac{\delta(s)}{\delta(t)}+\frac{\delta(t)}{\delta(s)}\right)$$

Several studies have focused on the inverse degree index and its extremal properties. Bojan Miti? et al. [6] established a set of inequalities that provide bounds for the inverse degree index of trees. Further developments were presented in [7], where additional inequalities were obtained and extremal graphs corresponding to the inverse degree index were characterized. That work also included a QSPR investigation of the inverse degree index along with its exponential extension. The extremal values of both the inverse degree index and the forgotten index within the class of unicyclic graphs were examined in [8]. Moreover, Muhammad Asif et al. [9] derived bounds for several families of connected n -vertex graphs containing pendant paths of fixed length attached to complete vertices, taking into account the effects of graph transformations. They also determined exact values of the inverse degree index for regular graphs, with particular emphasis on unicyclic structures. Building on these contributions, the present work establishes formulae for the degree inverse indices of transformation graphs.

Bounds on M_{DII}

In this section, we compute the bounds on M_{DII} for Ψ.

Theorem 2.1. Let ψ be a $(\theta,)$ – graph with ϵ pendant vertices and minimal non- pendant vertex degree η_1 . Then $M_{D\,I\,I}(\psi) \le \frac{2(\lambda-\epsilon)\mu^2+\epsilon(1+\mu^2)\eta_1^2}{\eta_1^4}$. Equality holds if and only if ψ (1,) – semiregular if $\epsilon\geq 0$ and ψ is regular if $\epsilon = 0$.

Proof. From the definition of MD_{II} we have

$$M_{D\,I\,I}(\psi) = \sum_{ts\in E(\psi)} \left(\frac{1}{\delta(t)^2}+\frac{1}{\delta(s)^2}\right)$$

$$= \sum_{ts\in E(\psi),\delta(t),\delta(s)\neq 1} \left(\frac{1}{\delta(t)^2}+\frac{1}{\delta(s)^2}\right) + \sum_{ts\in E(\psi),\delta(t)=1} \left(\frac{1}{1}+\frac{1}{\delta(s)^2}\right)$$

$$\leq \frac{2\mu^2}{\eta_1^4} \sum_{ts\in E(\psi),\delta(t),\delta(s)\neq 1} (1) + \frac{1+\mu^2}{\eta_1^2} \sum_{ts\in E(\psi),\delta(t)=1} (1)$$

$$= (\lambda-\epsilon)\frac{2\mu^2}{\eta_1^4} + \epsilon\frac{1+\mu^2}{\eta_1^2}$$

$$= \frac{2(\lambda-\epsilon)\mu^2+\epsilon\left(1+\mu^2\right)\eta_1^2}{\eta_1^4}$$

Equality holds if and only if Ψ $\delta(t) = \delta(s) = \eta_1$ for each non- pendant vertex $\dot{t}\boldsymbol{\varepsilon V}(\boldsymbol{\psi})$is regular. this implies ψ (1, μ) – semiregular if ∈≥ 0 and ψ is regular if ∈= 0.
If ψ has no pendant vertices then by previous theorem,

$$\mathrm{M}_{\mathrm{D\,II}}(\psi) = \frac{2\lambda\mu^2}{\eta^4}.$$

For a (θ,) – graph ψ, $\mathrm{M}_{\mathrm{D\,II}}(\psi) \leq \frac{2\lambda\mu^2}{\eta^4}$ Equality holds if and only if ψ is regular.

Proof. From the definition of $\mathrm{MD}_{\mathrm{II}}$ we have

$$\mathrm{M}_{\mathrm{D\,II}}(\psi) = \sum_{ts\in E(\psi)} \left(\frac{1}{\delta(t)^2} + \frac{1}{\delta(s)^2}\right) \tag{2.1}$$

For any t ∈ $V(\psi)$, $\eta \leq \delta(t) \leq \mu$. Thus

$$\mathrm{M}_{\mathrm{D\,II}}(\psi) \leq \frac{1}{\eta^4} \sum_{ts\in E(\psi)} (\delta(t)^2 + \delta(s)^2) \tag{2.2}$$

For any t ∈ $V(\psi)$, $\delta(t) \leq \theta - e(t)$. Thus

$$\mathrm{M}_{\mathrm{D\,II}}(\psi) \leq \frac{1}{\eta^4} \Sigma_{ts\in E(\psi)} ((\theta - e(t))^2 + (\theta - e(s))^2)$$

$$= \frac{1}{\eta^4} \sum_{ts\in E(\psi)} \left((\theta^2 + e(t)^2 - 2\theta e(t) + \theta^2 + e(s)^2 - 2\theta e(s)\right)$$

This gives that

$$\mathrm{M}_{\mathrm{D\,II}}(\psi) \leq \frac{2\lambda\mu^2}{\eta^4}$$

The eccentricity of a vertex t of Ψ is defined as maximum distance between t and all the vertices of Ψ. The eccentricity version of first Zagreb index and forgotten index of a graph Ψ are respectively defined as

$$\mathrm{ecc}_{\mathrm{FZI}}(\psi) = \sum_{ts\in E(\psi)} (e(t) + e(s))$$

and

$$\mathrm{ecc}_{\mathrm{FI}}(\psi) = \sum_{ts\in E(\psi)} (e(t)^2 + e(s)^2)$$

For a (θ,) – graph ψ, $\mathrm{M}_{\mathrm{D\,II}}(\psi) \leq \frac{2\theta^2}{\eta^4} + \frac{1}{\eta^4} ecc_{FI}(\psi) - \frac{2\theta}{\eta^4} ecc_{FZI}(\psi).$
Equality holds if and only if ψ is regular or biregular.
Proof. By the definition of $\mathrm{MD}_{\mathrm{II}}$, we have

$$M_{DII}(\psi) = \sum_{ts\in E(\psi)} \left(\frac{1}{\delta(t)^2} + \frac{1}{\delta(s)^2}\right) \qquad (2.1)$$

For any $t \in V(\psi)$, $\eta \le \delta(t) \le \mu$. Thus

$$M_{DII}(\psi) \le \frac{1}{\eta^4} \sum_{ts\in E(\psi)} (\delta(t)^2 + \delta(s)^2) \qquad (2.2)$$

For any $t \in V(\psi)$, $\delta(t) \le \theta - e(t)$. Thus

$$M_{DII}(\psi) \le \frac{1}{\eta^4}\Sigma_{ts\in E(\psi)}((\theta - e(t))^2 + (\theta - e(s))^2)$$

$$= \frac{1}{\eta^4} \sum_{ts\in E(\psi)} \left((\theta^2 + e(t)^2 - 2\theta e(t) + \theta^2 + e(s)^2 - 2\theta e(s)\right)$$

$$= \frac{1}{\eta^4} \sum_{ts\in E(\psi)} \left((2\theta^2 + (e(t)^2 + e(s)^2) - 2\theta(e(t) + e(s))\right)$$

This gives that

$$M_{DII}(\psi) \le \frac{2\theta^2}{\eta^4} + \frac{1}{\eta^4} \sum_{ts\in E(\psi)} (e(t)^2 + e(s)^2) - \frac{2\theta}{\eta^4} \sum_{ts\in E(\psi)} (e(t) + e(s))$$

By the definition of eccentricity version of forgotten index and first Zagreb index, we have

$$M_{DII}(\psi) \le \frac{2\theta^2}{\eta^4} + \frac{1}{\eta^4} ecc_{FI}(\psi) - \frac{2\theta}{\eta^4} ecc_{FZI}(\psi).$$

By the definition of eccentricity version of forgotten index and first Zagreb index, we have

$2\theta^2 1 2\theta$

$M_{DII}(\Psi) \le \quad \eta^4 + \eta^4 eccFI(\Psi) - \eta^4 eccFZI(\Psi).$

Transformation graph $R^{rs}(\Psi)$

The graph $R^{rs}(\Psi)$ is a graph with $V(R^{rs}(\Psi)) = (V(\Psi) \cup E(\Psi))$ such that two vertices r and s in $V(R^{rs}(\Psi))$ are adjacent if and only if the following holds

(i) $r, s \in V(\Psi)$, $rs \in E(\Psi)$ if $r = +$ and r and s are not adjacent if $r = -$.
(ii) $r \in V(\Psi)$ and $s \in E(\Psi)$, $rs \in E(\Psi)$ if $s = +$ and $rs \notin E(\Psi)$ if $s = -$.

One can observe that this transformation graph $R^{rs}(\Psi)$ has four graphs like $R^{++}(\Psi)$, $R^{+-}(\Psi)$, $R^{-+}(\Psi)$ and $R^{--}(\Psi)$.

Theorem 2.4. For a $(\theta, \lambda)-$ graph G, $R^{++}(S(\Psi)) =+ \underline{3\lambda}.$ $\frac{M_{DII}(\Psi)}{2}$ 4

Proof. By the definition of M_{DII} of $R^{++}(S(\Psi))$ we have

$$M_{DII}\left(R^{++}(S(\psi))\right) = \sum_{t\in V(R^{++}(S(\psi))} \frac{1}{\delta(t)}$$

From the structure of $R^{++}(S(\Psi))$, the number of vertices and edges are respectively, $\theta + 3\lambda$ and 6λ. In addition, the degree of $t \in V(R^{++}(S(\Psi))) \cap V(S(\Psi))$ is $2\delta(t)$ and degree of $ts \in V(R^{++}(S(\Psi))) \cap E(S(\Psi))$ is 2.
Hence,

$$M_{DII}\left(R^{++}(S(\psi))\right) = \sum_{t\in V\left(R^{++}(S(\psi))\cap V(S(\psi))\right)} \frac{1}{\delta(t)} + \sum_{ts\in V\left(R^{++}(S(\psi))\cap E(S(\psi))\right)} \frac{1}{\delta(t)}$$

$$= \sum_{t\in V(S(\psi))} \frac{1}{2\delta(t)} + \sum_{ts\in E(S(\psi))} \frac{1}{2}$$

$$= \sum_{t\in V(\psi)} \frac{1}{2\delta(t)} + \sum_{t\in V(S(\psi)/V(\psi))} \frac{1}{2\delta(t)} + \sum_{ts\in E(S(\psi))} \frac{1}{2}$$

$$= \frac{M_{DII}(\psi)}{2} + \frac{\lambda}{4} + \frac{\lambda}{2}$$

$$= \frac{M_{DII}(\psi)}{2} + \frac{3\lambda}{4}.$$

Theorem 2.5. For a $(\theta, \lambda)-$ graph G,

$$M_{DII}(R^{--}(S((\psi))) \leq \frac{\theta+\lambda}{4(\theta+3\lambda-1)} - \frac{M_{DII}(\psi)}{8} + \frac{\lambda}{4(\theta+3\lambda-1)} - \frac{\lambda}{16} + \frac{2\lambda}{\theta+\lambda-2}.$$

Proof. From the structure of $R^{--}(S(\Psi))$, it has $\theta + 3\lambda$ vertices and $2(\theta + \lambda)^2 - \lambda^2 - \theta$ edges. The degree of a vertex $t \in V(R^{--}(S(\Psi))) \cap V(S(\Psi))$ is $\theta + 3\lambda - 2\delta(t) - 1$ and an edge $ts \in V(R^{--}(S(\Psi))) \cap E(S(\Psi))$ is $\theta + \lambda - 2$. Thus

$$M_{DII}\left(R^{--}(S(\psi))\right) = \sum_{t\in V\left(R^{--}(S(\psi))\cap V(S(\psi))\right)} \frac{1}{\delta(t)} + \sum_{xy\in V\left(R^{--}(S(\psi))\cap E(S(\psi))\right)} \frac{1}{\delta(t)}$$

$$= \sum_{t\in V(S(\psi))} \frac{1}{\theta + 3\lambda - 2\delta(t) - 1} + \sum_{xy\in E(S(\psi))} \frac{1}{\theta + \lambda - 2}$$

$$= \sum_{t\in V(\psi)} \frac{1}{\theta + 3\lambda - 2\delta(t) - 1} + \sum_{t\in V(S(\psi)/V(\psi))} \left(\frac{1}{\theta + 3\lambda - 2\delta(t) - 1}\right)$$

$$+ \sum_{xy\in E(S(\psi))} \frac{1}{\theta + \lambda - 2}$$

By Jensen’s inequality, we have

$$\mathrm{M_{D\,I\,I}}\left(R^{--}(S(\psi))\right) \leq \frac{1}{4}\sum_{t\in V(\psi)}\left(\frac{1}{\theta+3\lambda-1}-\frac{1}{2\delta(t)}\right)+\sum_{t\in V(S(\psi)/V(\psi))}\left(\frac{1}{\theta+3\lambda-1}-\frac{1}{2\delta(t)}\right)$$

$$+\sum_{xy\in E(S(\psi))}\frac{1}{\theta+\lambda-2}$$

$$=\frac{\theta}{4(\theta+3\lambda-1)}-\sum_{t\in V(\psi)}\frac{1}{8\delta(t)}+\frac{\lambda}{4(\theta+3\lambda-1)}$$

$$-\sum_{t\in V(S(\psi)/V(\psi))}\frac{1}{16}+\frac{2\lambda}{\theta+\lambda-2}$$

$$=\frac{\theta+\lambda}{4(\theta+3\lambda-1)}-\frac{M_{DII}(\psi)}{8}+\frac{\lambda}{4(\theta+3\lambda-1)}-\frac{\lambda}{16}+\frac{2\lambda}{\theta+\lambda-2}.$$

Theorem 2.6. For a $(\theta,)$ − graph with G, $M_{DII}(R^{+-}S(\psi)) = \frac{\lambda+\theta}{2\lambda}+\frac{2\lambda}{\theta+\lambda-2}.$

Proof.

$$\mathrm{M_{DII}}(\mathrm{R}^{+-}\mathrm{S}(\psi)) = \sum_{t\in V\left(R^{+-}(S(\psi))\right)}\frac{1}{\delta(t)}.$$

From the construction of the graph (R+ −(S(ψ)), the number of vertices and edges of (R+ −(S(ψ)) are respectively θ+3λ and (θ+λ)2 − 2λ. Likewise, the degree of a vertex t ∈ V(R+ −(S(ψ))) ∩ V(S(ψ) is 2λ and an edge t s ∈ V(R+ −(S(ψ))) ∩ E(S(ψ) is θ+λ −2 .
Hence,

$$M_{DII}(R^{+-}S(\psi)) = \sum_{t\in V\left(R^{+-}(S(\psi))\cap V(S(\psi))\right)}\frac{1}{\delta(t)}+\sum_{ts\in V\left(R^{+-}(S(\psi))\cap E(S(\psi))\right)}\frac{1}{\delta(t)}$$

$$=\sum\nolimits_{t\in E(S(\psi))}\frac{1}{2\lambda}+\sum\nolimits_{ts\in E(S(\psi))}\frac{1}{\theta+\lambda-2}$$

$$=\sum_{t\in V(S(\psi)/V(\psi))}\frac{1}{2\lambda}+\sum_{t\in V(\psi)}\frac{1}{2\lambda}+\sum_{ts\in E(S(\psi))}\frac{1}{\theta+\lambda-2}$$

$$=\frac{\lambda}{2\lambda}+\frac{\theta}{2\lambda}+\frac{2\lambda}{\theta+\lambda-2}$$

$$M_{DII}(R^{+-}S(\psi)) = \frac{\lambda+\theta}{2\lambda}+\frac{2\lambda}{\theta+\lambda-2}\ .$$

Theorem 2.7. For a (θ, λ)− graph G , $M_{DII}(R^{-+}S(\psi)) = \frac{\lambda+\theta}{\theta+\lambda-1}+\lambda.$

Proof. From the structure of R^{-+}(S(Ψ)) , the number of vertices and edges are θ + 3λ and (θ +λ)(θ +λ−1) respectively. In addition, the degree of a vertex t ∈ V (R^{-+}(S(Ψ))) is θ + λ − 1 and an edge ts ∈ V (Ψ) ∩ E(S(Ψ)) is 2 . Thus,

$$M_{DII}(R^{-+}S(\psi)) \;=\; \sum_{t\in V\left(R^{-+}(S(\psi))\cap V(S(\psi))\right)} \frac{1}{\delta(t)} + \sum_{ts\in V\left(R^{-+}(S(\psi))\cap E(S(\psi))\right)} \frac{1}{\delta(t)}$$

$$= \sum_{t\in V(S(\psi))} \frac{1}{\theta+\lambda-1} + \sum_{ts\in E(S(\psi))} \frac{1}{2}$$

$$= \sum_{t\in V(S(\psi))/V(\psi)} \frac{1}{\theta+\lambda-1} + \sum_{t\in V(\psi)} \frac{1}{\theta+\lambda-1} + \sum_{ts\in E(S(\psi))} \frac{1}{2}$$

$$= \frac{\lambda}{\theta+\lambda-1} + \frac{\theta}{\theta+\lambda-1} + \frac{2\lambda}{2}$$

$$= \frac{\lambda+\theta}{\theta+\lambda-1} + \lambda.$$

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