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Research Article

On the extremal total irregularity index of n-vertex trees with fixed maximum degree

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Abstract: In the extension of irregularity indices, Abdo et. al. [H. Abdo, S. Brandt, D. Dimitrov, The total irregularity of a graph, Discrete Math. Theor. Comput. Sci. **16** (2014), 201–206] defined the total irregularity of a graph $G = (V, E)$ as $irr_t(G) = \frac{1}{2}\sum_{u,v\in V(G)} \left|d_u - d_v\right|$, where d_u denotes the vertex degree of a vertex $u \in V(G)$. In this paper, we investigate the total irregularity of trees with bounded maximal degree Δ and state integer linear programming problem which gives standard information about extremal trees and it also calculates the index.

Keywords: Irregularity, total irregularity index, maximal degree, molecular trees, integer linear programming problem

AMS Subject classification: 05C09, 05C92

1. Introduction

In the present paper notation $G = (V, E)$ represent a simple, connected, undirected and finite graph. Chemical compounds are represented by molecular graphs in which atoms represented by nodes (vertices) and covalent bonds are represented by lines (edges). Saturated hydrocarbons and alkanes are examples of molecular graphs. Maximal degree of graph G is denote by $\Delta(G)$. In CGT (chemical graph theory), if the maximum degree of a graph is 4, then it is called a molecular graph. If vertex set of G is $\{v_1, v_2, \ldots, v_n\}$, then the sequence $\langle d_{v_1}, d_{v_2}, \ldots, d_{v_n}\rangle$ is called a $\mathbb{DS}$ (degree

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sequence) of G [12, 14]. In addition, the term $D(G) = [z_1^{t_1}, z_2^{t_2}, \ldots, z_p^{t_p}]$ explains that the $\mathbb{DS}$ (degree sequence) contains t_i vertices of degree z_i where $i = 1, 2, \ldots, p$. For further basic notation and terminology not explained here, we refer the reader to [11, 12, 14].

If every vertex of a graph(molecular) has the same degree, then it is said to be *regular*, otherwise the graph is *irregular*. Many graph invariants (topological indices) are proposed to measure the irregularity [3–6, 13, 15, 16, 19], their application in chemistry, in particular in QSPR and QSAR can be seen in [7, 9, 10].

Abdo et. al. [1] extend the work of Albertson by proposing a new irregularity measure the total irregularity, denoted by $irr_t(G)$ and defined as

$$irr_t(G) = \frac{1}{2} \sum_{(u,v)\in V^2(G)} \left| d_u - d_v \right|. \tag{1}$$

Mathematical application of total irregularity index can be seen in [1, 2, 8, 17, 18, 20]. If one of the vertex of a tree is nominated as a root, then the tree is said to be *rooted*. *Parent* of a vertex is defined as the vertex that immediately prior to it on the path to the root. If a subtree is connected to a vertex t, then t (vertex) is called parent of a subtree. If w_1 is the parent of w_2, then w_2 is called *child* vertex. In this paper, we characterize the structure of trees with maximum degree Δ that have maximum $irr_t - value$.

2. Main Result

To establish the main result, we use the following transformation. We use the notation $\mathbb{RT}$ for rooted tree and t_i the number of vertices of $\mathbb{RT}$ of degree i, for each $i = 1, 2, \ldots, \Delta$.

Transformation 2.1. *Suppose that $v \in \mathbb{RT}$ is designated as a root with degree Δ. Suppose that $\mathbb{RT}$ is composed of vertices of maximum degrees (Δ), pendent vertices and in certain cases another vertex v_1, with $2 \le d_{v_1} \le \Delta - 1$. Denote by Ω the collection of all vertices of $\mathbb{RT}$ whose degrees are in the interval $[2, \Delta - 1]$. Let $d_{v_1} \ge \ldots \ge d_{v_k}$ be the order of the degrees of vertices in Ω. Construct $\acute{\mathbb{RT}} = \mathbb{RT} - v_k w + v_1 w$, where v_k is a parent vertex of w.*

Lemma 1. *Let $\acute{\mathbb{RT}}$ be a tree that is obtained after applying Transformation 2.1. It holds that*

$$irr_t(\mathbb{RT}) - irr_t(\acute{\mathbb{RT}}) < 0.$$

Proof. After applying Transformation 2.1, the pair (d_{v_1}, d_{v_k}) will be changed by $(d_{v_1} + 1, d_{v_k} - 1)$ and set Ω will be replaced by $\acute{\Omega}$. For $i = 1, 2, \ldots, \Delta$, let V_i be the set of vertices with degree i in $\mathbb{RT}$. If $A = \bigcup_{i=1}^{\Delta-1} V_i$ and $B = \bigcup_{i=2}^{\Delta} V_i$ then bearing in mind the assumptions that d_{v_1} and d_{v_k} are the second maximum and second minimum degrees of T respectively and that $\sum_{i=2}^{\Delta-1} t_i \geq 2$, we have

$$\begin{aligned}
irr_t(T) - irr_t(\acute{T}) &= (d_{v_1} - d_{v_k}) - ((d_{v_1}+1) - (d_{v_k}-1)) \\
&\quad + \sum_{x\in A\setminus\{v_1,v_k\}} ((d_{v_1} - d_x) - (d_{v_1} + 1 - d_x)) \\
&\quad + t_\Delta \left[(\Delta - d_{v_1}) - (\Delta - (d_{v_1}+1))\right] \\
&\quad + t_1 \left[(d_{v_k} - 1) - (d_{v_k} - 1 - 1)\right] \\
&\quad + \sum_{y\in B\setminus\{v_1,v_k\}} ((d_y - d_{v_k}) - (d_y - (d_{v_k} - 1))) \\
&= -2 - \left(\sum_{i=1}^{\Delta-1} t_i - 2\right) + t_\Delta + t_1 - \left(\sum_{i=2}^{\Delta} t_i - 2\right) \\
&= 2 - 2\sum_{i=2}^{\Delta-1} t_i < 0.
\end{aligned}$$

□

Remark 1. From Transformation 2.1, we have $|\acute{\Omega}| \leq |\Omega|$, with (strict) inequality if $d_{v_k} = \Delta - 1$ or $d_{v_1} = 2$. If the cardinality of $\acute{\Omega}$ is greater or equal to 2, we select a vertex with maximum degree and a vertex with minimum degree from $\acute{\Omega}$ and repeat the Transformation 2.1 continuously to get $|\acute{\Omega}| = 1$ or $|\acute{\Omega}| = 0$. It holds that $\mathbb{DS}$ of $\mathbb{RT}$ is $[\Delta^{t_\Delta}, 1^{t_1}]$ or $[\Delta^{t_\Delta}, z^1, 1^{t_1}]$, $2 \leq z \leq \Delta - 1$.

Theorem 1. *Let $\mathbb{RT}$ be a tree with maximal total irregularity index and maximum degree Δ. Then:*
(i) If $n = 2 + (\Delta-1)q$ where $q \in \mathbf{Z}$, then $\mathbb{RT}$ consists of $\frac{n-2}{\Delta-1}$ vertices of degree Δ and $\frac{n(\Delta-2)+2}{\Delta-1}$ pendent vertices.
(ii) If $n = 1 + z + (\Delta-1)q$ where $q \in \mathbf{Z}$, then $\mathbb{RT}$ consists $\frac{n-1-z}{\Delta-1}$ vertices of degree Δ and $\frac{(n-1)(\Delta-2)+z}{\Delta-1}$ pendent vertices and one vertex of degree z where $2 \leq z \leq \Delta - 1$.

Proof. Suppose that $v \in \mathbb{RT}$ is designated as a root and $d_v = \Delta$. Denote by t_i the number of vertices of $\mathbb{RT}$ of degree i, for each $i = 1, 2, \ldots, \Delta$. Using Transformation 2.1, Lemma 1 and Remark 1, it follows that $\mathbb{RT}$ has a $\mathbb{DS}$ $[\Delta^{t_\Delta}, 1^{t_1}]$ or $[\Delta^{t_\Delta}, z^1, 1^{t_1}]$, $2 \leq z \leq \Delta - 1$.
There will be two cases regarding to the cardinality of $|\Omega|$, in which we find the values of t_Δ, t_1 and z.

Case 1. If $|\Omega| = 0$, then the $\mathbb{DS}$ of $\mathbb{RT}$ is $[\Delta^{t_\Delta}, 1^{t_1}]$ and the following well-known equations

$$\sum_{i=1}^{\Delta} t_i \;=\; t_\Delta + t_1 = n \tag{2}$$

and

$$\sum_{i=1}^{\Delta} it_i \;=\; \Delta t_\Delta + t_1 = 2(n-1) \tag{3}$$

holds. Solving the equations (2) and (3), we get

$$t_\Delta = \frac{n-2}{\Delta-1}, \quad t_1 = \frac{n(\Delta-2)+2}{\Delta-1} \quad \text{for } n = 2 + (\Delta-1)q.$$

Case 2. If $|V_\alpha| = 1$, then the $\mathbb{DS}$ of $\mathbb{RT}$ is $[\Delta^{t_\Delta}, z^1, 1^{t_1}]$ along with

$$\sum_{i=1}^{\Delta} t_i \;=\; t_\Delta + t_1 + 1 = n \tag{4}$$

and

$$\sum_{i=1}^{\Delta} it_i \;=\; \Delta t_\Delta + t_1 + z = 2(n-1). \tag{5}$$

Solving the equations (4) and (5), we get

$$t_\Delta = \frac{n-1-z}{\Delta-1}, \quad t_1 = \frac{(n-1)(\Delta-2)+z}{\Delta-1} \quad \text{for } n = 1 + z + (\Delta-1)q.$$

□

As a direct result of Theorem 1, we will get the maximum $irr_t - value$ for $\mathbb{RT}$ trees with maximum degree Δ.

Corollary 1. *Let $\mathbb{RT}$ be a tree with maximum total irregularity index among the trees with n vertices and maximum degree Δ.*
(i) If $n = 2 + (\Delta-1)q$ where $q \in \mathbf{Z}$, then

$$irr_t(T) = \frac{(n-2)(n(\Delta-2)+2)}{\Delta-1}.$$

(ii) If $n = 1 + z + (\Delta - 1)q$ *where* $q \in \mathbf{Z}$*, then*

$$irr_t(T) = \frac{1}{\Delta - 1}[(n-1)(n-2)(\Delta - 2) + (n-1)\Delta - z(\Delta + 1) + z^2].$$

where $2 \leq z \leq \Delta - 1$.

Proof. (*i*) If $n = 2 + (\Delta - 1)q$ where $q \in \mathbf{Z}$, by Theorem 1, the $\mathbb{DS}$ of $\mathbb{RT}$ is $[\Delta^{t_\Delta}, 1^{t_1}]$ where $t_\Delta = \frac{n-2}{\Delta-1}$ and $t_1 = \frac{n(\Delta-2)+2}{\Delta-1}$. Thus,

$$irr_t(T) = (\Delta - 1) \cdot \frac{n-2}{\Delta - 1} \cdot \frac{n(\Delta - 2) + 2}{\Delta - 1}$$

or

$$irr_t(T) \;=\; \frac{(n-2)(n(\Delta - 2) + 2)}{\Delta - 1}. \tag{6}$$

(*ii*) Otherwise, T has $\mathbb{DS}$ $[\Delta^{t_\Delta}, z^1, 1^{t_1}]$ with $t_1 = \frac{(n-1)(\Delta-2)+z}{\Delta-1}$ and $t_\Delta = \frac{n-1-z}{\Delta-1}$. Thus,

$$\begin{aligned} irr_t(T) = (\Delta - 1) \cdot \frac{n-1-z}{\Delta - 1} \cdot \frac{(n-1)(\Delta - 2) + z}{\Delta - 1} + (\Delta - z) \cdot \frac{n-1-z}{\Delta - 1} \\ + (z-1) \cdot \frac{(n-1)(\Delta - 2) + z}{\Delta - 1}. \end{aligned}$$

Hence,

$$irr_t(T) \;=\; \frac{1}{\Delta - 1}[(n-1)(n-2)(\Delta - 2) + (n-1)\Delta - z(\Delta + 1) + z^2]. \tag{7}$$

□

Theorem 2. *Let* $\mathbb{MT} \in \mathbb{RT}$ *be a chemical (molecular) tree with maximum total irregularity index among the trees with* n *vertices. Then, we have:*
(i)If $n = 2 + 3q$ *where* $q \in \mathbf{Z}$*, then the* $\mathbb{DS}$ *of* $\mathbb{MT}$ *is* $[4^{\frac{n-2}{3}}, 1^{\frac{2n+2}{3}}]$*. Its total irregularity index is*

$$irr_t(\mathbb{MT}) = \frac{2(n+1)(n-2)}{3}.$$

(ii)If $n = 1 + z + 3q$ *where* $q \in \mathbf{Z}$*, then the* $\mathbb{DS}$ *of* $\mathbb{MT}$ *is* $[4^{\frac{n-1-z}{3}}, z^1, 1^{\frac{2(n-1)+z}{3}}]$*, where* $2 \leq z \leq 3$*. Its total irregularity index is*

$$irr_t(\mathbb{MT}) = \frac{1}{3}[2n(n-1) + z(z-5)].$$

Proof. For $2 \leq n \leq 5$, the S_n (star graph) maximizes the total irregularity index [1]. For $n = 6$ and $\Delta \leq 4$, the possible $\mathbb{DS}$ of $\mathbb{MT}$ are $[2^4, 1^2]$, $[3^1, 2^2, 1^3]$, $[3^2, 2^1, 1^3]$ and $[4^1, 2^1, 1^4]$. The last of these $\mathbb{DS}$ corresponds to the maximum total irregularity index. Thus, the theorem is satisfied for $2 \leq n \leq 6$.

Now, we assume that $n \geq 7$. A tree with maximum degree Δ is denoted by $\mathbb{MT}_\Delta$. Since $\mathbb{MT}$ is a chemical (molecular) tree. By Corollary 1(i), $irr_t(\mathbb{MT}_2) = 2n - 4$. Further, we consider the following two cases:

Case 1. Consider $n = 2 + 2q$ where $q \in \mathbf{Z}$. By Corollary 1(i), we have $irr_t(\mathbb{MT}_3) = \frac{n^2-4}{2}$. Since $n = 2 + 2q$, it follows that $n \neq 2 + 3q$ where $q \in \mathbf{Z}$, and by Corollary 1(ii), $irr_t(\mathbb{MT}_4) = \frac{1}{3}[2n(n-1) + z(z-5)]$ where $z = 2$ or $z = 3$. For $n \geq 7$, by simplification one can see that $irr_t(\mathbb{MT}_4) > irr_t(\mathbb{MT}_3) > irr_t(\mathbb{MT}_2)$ is satisfied.

Case 2. Consider $n \neq 2+2q$ where $q \in \mathbf{Z}$. By Corollary 1 (ii), we have $irr_t(\mathbb{MT}_3) = \frac{1}{2}[n^2 - 1 + z(z-4)]$ where $z = 2$ or $z = 3$. We distinguish two situations.
Subcase 2.1. Consider $n = 2 + 3q$ where $q \in \mathbf{Z}$. By Corollary 1(i), we have $irr_t(\mathbb{MT}_4) = \frac{2(n+1)(n-2)}{3}$. For $n \geq 7$, and $z = 2, 3$, it holds that $irr_t(\mathbb{MT}_4) > irr_t(\mathbb{MT}_3) > irr_t(\mathbb{MT}_2)$.

Subcase 2.2. Consider $n \neq 2 + 3q$ where $q \in \mathbf{Z}$. By Corollary 1 (ii), we have $irr_t(\mathbb{MT}_4) = \frac{1}{3}[2n(n-1) + z(z-5)]$. Again, a direct calculation results that $irr_t(\mathbb{MT}_4) > irr_t(\mathbb{MT}_3) > irr_t(\mathbb{MT}_2)$.
Hence proved. □

Alternatively, a complete characterization of Theorem 1 can be obtained by solving the following integer linear programming problem. The number of vertices of tree $\mathbb{RT}$ of degree i is denoted by t_i, for all $1 \leq i \leq \Delta$ and the number of edges joining a vertex of degree i with a vertex of degree j, is denoted by m_{ij}.

Integer Linear Programming Problem:

Let T be a tree with maximum total irregularity index among all trees with n vertices and maximum degree Δ. Then, the trees with maximum total irregularity index are completely represented by solving the maximization problem:

$$\text{Max } \ irr_t(T) = \sum_{i,j=1}^{\Delta} \frac{1}{2}\big|i - j\big| t_i t_j$$

$$\text{sub. to } \sum_{i=1}^{\Delta} t_i = n$$

$$\sum_{i=1}^{\Delta} it_i = 2(n-1),$$

$$\sum_{i=2}^{\Delta-1} t_i \leq 1,$$

$$\sum_{i,j=1,j\neq i}^{\Delta} m_{ij} + 2m_{ii} = it_i$$

where $0 \leq t_i \leq n-1$, $1 \leq i \leq \Delta$ and $0 \leq m_{ij} \leq n-2$, $1 \leq i, j \leq \Delta$.

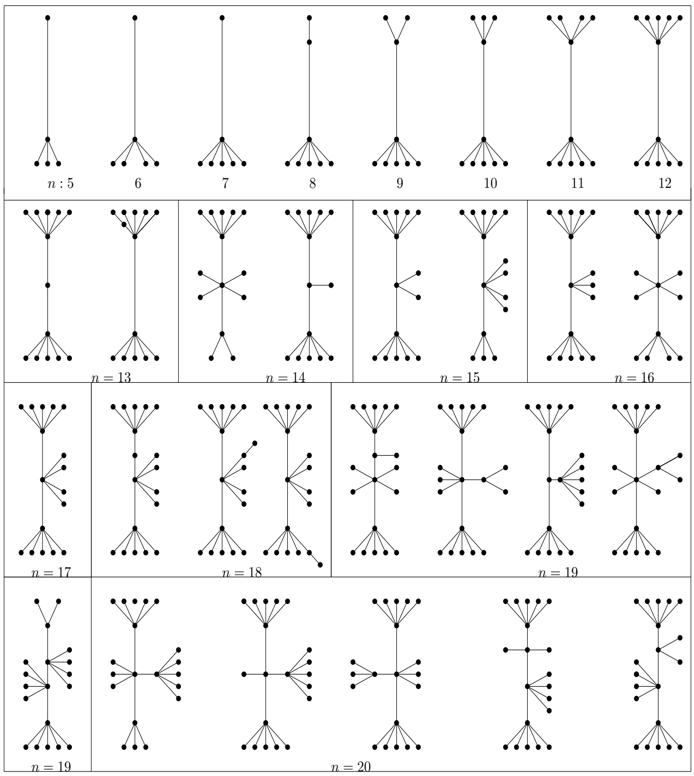

Figure 1. Extremal trees of orders $n = 5, 6, \ldots, 20$, $\Delta = 6$ with respect to the total irregularity index.

Concluding Remark: In the present study, we determine that Caterpillar has maximum total irregularity index among all n-vertex trees having maximum degree Δ.

Figure 1 represents extremal trees with maximum degree 6. Finally, Integer Linear Programming Problem of extremel trees is also stated.

References

[1] H. Abdo, S. Brandt, and D. Dimitrov, *The total irregularity of a graph*, Discrete Math. Theor. Comput. Sci. **16** (2014), no. 6, 201–206.

[2] H. Abdo and D. Dimitrov, *The total irregularity of graphs under graph operations*, Miskolc Math. Notes **15** (2014), no. 1, 3–17.

[3] M.O. Albertson, *The irregularity of a graph*, Ars Combin. **46** (1997), 219–225.

[4] A.R. Ashrafi, A. Ghalavand, and A. Ali, *Molecular trees with the sixth, seventh and eighth minimal irregularity values*, Discrete Math. Algorithms Appl. **11** (2019), no. 1, 1950002.

[5] F.K. Bell, *A note on the irregularity of graphs*, Linear Algebra Appl. **161** (1992), 45–54.

[6] L. Collatz and U. Sinogowitz, *Spektren endlicher grafen*, Abh. Math. Sem. Univ. Hamburg, vol. 21, Springer, 1957, pp. 63–77.

[7] R. Criado, J. Flores, A.G. del Amo, and M. Romance, *Centralities of a network and its line graph: an analytical comparison by means of their irregularity*, Int. J. Comput. Math. **91** (2014), no. 2, 304–314.

[8] D. Dimitrov and R. Škrekovski, *Comparing the irregularity and the total irregularity of graphs*, Ars Math. Contemp. **9** (2014), no. 1, 45–50.

[9] E. Estrada, *Quantifying network heterogeneity*, Phys. Rev. E **82** (2010), no. 6, ID: 066102.

[10] ______, *Randić index, irregularity and complex biomolecular networks*, Acta Chim. Slov. **57** (2010), no. 3, 597–603.

[11] E. Estrada and D. Bonchev, *Section 13.1. Chemical Graph Theory*, Handbook of Graph Theory (2013), 1538–1558.

[12] J.L. Gross and J. Yellen, *Graph Theory*, CRC Press,Boca Raton, Florida, 2000.

[13] I. Gutman, P. Hansen, and H. Mélot, *Variable neighborhood search for extremal graphs. 10. comparison of irregularity indices for chemical trees*, J. Chem. Inf. Model. **45** (2005), no. 2, 222–230.

[14] F. Harary, *Graph Theory*, Addison-Wesley, 1969.

[15] T. Réti and A. Ali, *On the variance-type graph irregularity measures*, Commun. Comb. Optim. **5** (2020), no. 2, 169–178.

[16] T. Réti, R. Sharafdini, A. Drégelyi-Kiss, and H. Haghbin, *Graph irregularity indices used as molecular descriptors in QSPR studies*, MATCH Commun. Math. Comput. Chem. **79** (2018), no. 2, 509–524.

[17] L. You, J. Yang, and Z. You, *The maximal total irregularity of unicyclic graphs*, Ars Combin. **114** (2014), 153–160.

[18] L. You, J. Yang, Y. Zhu, and Z. You, *The maximal total irregularity of bicyclic*

graphs, J. Appl. Math. **2014** (2014), ID: 785084.

[19] S. Yousaf, A.A. Bhatti, and A. Ali, *A note on the modified Albertson index*, Util. Math. (to appear).

[20] Y. Zhu, L. You, and J. Yang, *The minimal total irregularity of some classes of graphs*, Filomat **30** (2016), no. 5, 1203–1211.