MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **76** (2016) 649-657

ISSN 0340 - 6253

Partial Orderings of Trees According to Zagreb Indices

John Estes[a], Emlee Nicholson[b], Bing Wei[c]

[a]*Department of Mathematics, Belhaven University, Jackson, Mississippi*
jestes@belhaven.edu

[b]*Department of Mathematics, Millsaps College, Jackson, Mississippi*
nichoe@millsaps.edu

[c]*Department of Mathematics, University of Mississippi, University, Mississippi*
bwei@olemiss.edu

(Received March 7, 2016)

Abstract

The first and second Zagreb indices, M_1 and M_2, respectively are defined as follows: $M_1 = \sum_{v\in V(G)}(d(v))^2$ and $M_2 = \sum_{uv\in E(G)}(d(v)d(u))$. For a given tree T, we will build a finite sequence of trees $\{T_i\}_0^k$ where $T_0 \cong P_n$, $T_k \cong S_n$, and T is in this sequence. Such a sequence will be termed a genealogy of T. Furthermore, under certain parameters, $F(T_i) \leq F(T_{i+1})$ for $F \in \{M_1, M_2\}$.

1 Introduction

We will consider only simple undirected graphs. For any graph G, we use $V(G)$ or V to denote its vertex set and $E(G)$ or E to denote its edge set. We denote $N(u)$ to be the set of neighbors of $u \in V(G)$, $N[u] = N(u) \cup \{u\}$, $d_G(v) = |N(v)|$ for the degree of $v \in V(G)$, and for $S \subseteq V$, we denote $\sum_{v\in S} d(v)$ by $d(S)$. For the tree T, we define the set of leaves as $S_1(T) = \{v \in V(T)|d_T(v) = 1\}$. Let $T_1 = T - S_1(T)$ and set $S_2 = S_1(T_1)$. The first and second Zagreb indices, M_1 and M_2 respectively, are defined as follows:

(i) $M_1 = \sum_{v\in V(G)}(d(v))^2$

(ii) $M_2 = \sum_{uv\in E(G)}(d(v)d(u))$.

In 1975, Randić introduced the branching index which later became known as the Randić connectivity index [12]. The Randić connectivity index is mostly used as a molecular descriptor in computational chemistry describing nonempirical quantitative structure-property relationships and quantitative structure-activity relationships [7]. However, mathematicians have also expressed interest in the Randić connectivity index [1].

The Randić connectivity index has been generalized as the general Randić connectivity index and the general zeroth-order Randić connectivity index, where the Zagreb indices appeared as a special case [2]. The first Zagreb index $M_1(G)$ and the second Zagreb index $M_2(G)$ of the graph G are given by:

$$M_1(G) = \sum_{u \in V(G)} d(u)^2, \qquad M_2(G) = \sum_{uv \in E(G)} d(u)d(v).$$

The Zagreb indices M_1 and M_2 have been an active area of research going back to 1972 in the report of Gutman and Trinajstić in computational chemistry [9].

In regards to the Zagreb indices, there are two classical problems which have attracted the attention of researchers for some time:

(i) How $M_1(G)$ (respectively $M_2(G)$) depends on the structure of G.

(ii) Given a set of graphs $\mathcal{G}$, find upper and lower bounds for $M_1(G)$ and $M_2(G)$ of graphs in $\mathcal{G}$ and characterize the graphs in which the maximal (respectively minimal) M_1-, M_2-values are attained.

There have been numerous studies in the literature of the properties of Zagreb indices of given graph classes [4, 6, 10, 11]. In particular, Das and Gutman in 2004 characterized the Zagreb indices for trees and determined the unique tree that obtains minimum M_1 and M_2 values respectively, as well as maximum M_1 and M_2 values respectively.

Theorem 1. *[5][8] Let T be any tree of order n, and let P_n and S_n be the path and star respectively on n vertices. Then*

(i) $4n-6 \leq M_1(T) \leq n^2-n$, the left equality holds if and only if $T \cong P_n$, and the right equality holds if and only if $T \cong S_n$.

(ii) $4n-8 \leq M_2(T) \leq n^2-2n+1$, the left equality holds if and only if $T \cong P_n$ and the right equality holds if and only if $T \cong S_n$.

In 2013, Csikvári introduced the generalized tree shift, that when applied to a tree T to yield tree T', shows the largest eigenvalues of the adjacency matrix and Laplacian matrix of T are less than those in T'. Similar results are provided for characteristic polynomials, independence polynomials, and edge cover polynomials. From this, Csikvári built a partially ordered set of trees with respect to these respective indices for a given tree T starting with the path and ending with the star [3].

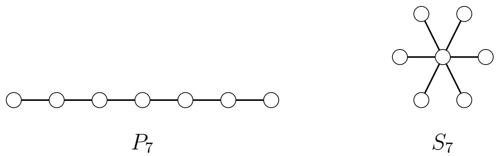

Figure 1: The path and star on 7 vertices

From the results of Das and Gutman, we see that a given tree T has values of M_1 and M_2 somewhere in between the respective values of P_n and S_n. We consider comparing these indices for trees T_1, $T_2 \notin \{P_n, S_n\}$. Can we relate $M_1(T_1)$ and $M_1(T_2)$? To answer these questions, we utilize the results of the following discussion in the spirit of the works of Csikvári.

2 Tree Genealogies

For a given tree T, we will build a finite sequence of trees $\{T_i\}_0^k$ where $T_0 \cong P_n$, $T_k \cong S_n$, and T is in this sequence. Furthermore, under certain parameters, $F(T_i) \leq F(T_{i+1})$ for $F \in \{M_1, M_2\}$. Such a sequence will be termed a genealogy of T.

First, we define a starring triple as follows: Let $r = \{v, u, x\}$ be such that

(i) $v \in S_1(T)$

(ii) the vu-path P is of length l,

(iii) for any $y \in P - \{v, u\}$, $d(y) = 2$,

(iv) $x \in V(T) - P$.

Let $R_l(T)$ be the set of such triples for a fixed l. For $r \in R_l(T)$, $T(r)$ is the tree with $V(T(r)) = V(T)$ and $E(T(r)) = (E(T) \cup \{yx\}) - \{yu\}$ where $y \in N(u) \cap V(P)$ (If $l = 1$, then $y = v$.). Let $R = \bigcup R_l$ over all $1 \leq l \leq n-1$.

Define

(i) $g : R \to \mathbb{Z}$ such that $g(r) = d(x) - d(u)$.

(ii) $h : R \to \mathbb{Z}$ such that $h(r) = d(N[x]) - d(N[u])$.

(iii) $r_\Delta = |N[x] \cap N[u]| - |N(x) \cap N(u)|$

(iv) $f : R \to \mathbb{Z}$ such that $f(r) = h(r) - \frac{1}{2}r_\Delta$ if $r \in R_1$ and $f(r) = g(r) + h(r) - \frac{1}{2}r_\Delta$ if $r \in R - R_1$.

If $g(r) > -1$, then $T(r)$ is said to be an l-descendant of T with respect to g. If $g(r) < -1$, then $T(r)$ is said to be an l-ancestor of T with respect to g. Let $k = -2$ if $l = 1$ and $k = -4$ if $l > 1$. If $f(r) > k$, then $T(r)$ is said to be an l-descendant of T with respect to f. If $f(r) < k$, then $T(r)$ is said to be an l-ancestor of T with respect to f. We first demonstrate the relationship between ancestors and descendants.

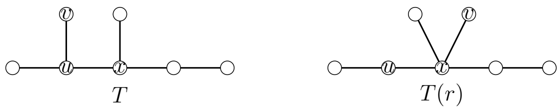

Figure 2: A tree T and $T(r)$

Theorem 2. *Let T and T' be trees and $j \in \{f, g\}$. Then T is an l-ancestor of T' with respect to j if and only if T' is an l-descendant of T with respect to j.*

Proof. (i) Let $r = \{v, u, x\} \in R(T)$, and suppose $g(r) > -1$. Then $T(r)$ is an l-descendant of T with respect to g, and $r' = \{v, x, u\} \in R(T(r))$. Note that $T(r)(r') \cong T$. Now $d_{T(r)}(u) = d_T(u) - 1$ and $d_{T(r)}(x) = d_T(x) + 1$. Thus $g(r') = d_{T(r)}(u) - d_{T(r)}(x) = d_T(u) - d_T(x) - 2 < -1$. Thus T is an l-ancestor of $T(r)$. The argument is reversible to show that if $T(r)$ is an l-ancestor of T with respect to g, then T is an l-descendant of $T(r)$ with respect to g.

(ii) Let $r = \{v, u, x\} \in R(T)$ and $l = 1$, and suppose $f(r) > -2$. Then $T(r)$ is an 1-descendant of T with respect to f. Let $r' = \{v, x, u\} \in R(T(r))$. Note that $T(r)(r') \cong T$. As $N_{T(r)}[x] = N_T[x] \cup v$, $N_{T(r)}[u] = N_T[u] - v$ and $d_T(v) = 1$,
if $x \notin N(u)$, then $r_\Delta = 0$, $d(N_{T(r)}[u]) = d(N_T[u]) - 2$ and $d(N_{T(r)}[x]) = d(N_T[x]) + 2$. Thus $d(N_{T(r)}[u]) - d(N_{T(r)}[x]) - \frac{1}{2}r_\Delta \leq -(d(N_T[x]) - d(N_T[u]) - \frac{1}{2}r_\Delta) - 2 - 2 - 0 < 2 - 4 = -2$. If

$x \in N(u)$, then $r_\Delta = 2$, $d(N_{T(r)}[u]) = d(N_T[u]) - 1$ and $d(N_{T(r)}[x]) = d(N_T[x]) + 1$. Thus $d(N_{T(r)}[u]) - d(N_{T(r)}[x]) - \frac{1}{2}r_\Delta \leq -(d(N_T[x]) - d(N_T[u]) - \frac{1}{2}r_\Delta) - 1 - 1 - 2 < 2 - 4 = -2$. Thus $f(r') < -2$. Hence T is a 1-ancestor of $T(r)$ with respect to f. The argument is reversible to show that if $T(r)$ is a 1-ancestor of T with respect to f, then T is a 1-descendant of $T(r)$ with respect to f.

Suppose $r = \{v, u, x\} \in R(T)$ and $l > 1$ and $f(r) > -4$. Then $T(r)$ is an l-descendant of T with respect to f. So $f(r) = g(r) + h(r) - \frac{1}{2}r_\Delta = d_T(x) - d_T(u) + d(N_T[x]) - d(N_T[u]) - \frac{1}{2}r_\Delta > -4$.

Let $r' = \{v, x, u\} \in R(T(r))$. Note that $T(r)(r') \cong T$. Now $f(r') = g(r') + h(r') - \frac{1}{2}r'_\Delta = d_{T(r)}(u) - d_{T(r)}(x) + d(N_{T(r)}[u]) - d(N_{T(r)}[x]) - \frac{1}{2}r_\Delta$.

Note that when $ux \in E(T)$, $r_\Delta = 2$ and $d(N_{T(r)}[u]) = d(N_T[u]) - 2$ while $d(N_{T(r)}[x]) = d(N_T[x]) + 2$. Thus when $ux \in E(T)$, $f(r') = -(d_T(x) - d_T(u) + d(N_T[x]) - d(N_T[u]) - \frac{1}{2}r_\Delta - 1 - 1 - 2 - 2 - 2 < 4 - 8 = -4$. Thus $f(r') < -4$.

Note that when $ux \notin E(T)$, $r_\Delta = 0$ and $d(N_{T(r)}[u]) = d(N_T[u]) - 3$ while $d(N_{T(r)}[x]) = d(N_T[x]) + 3$. Thus when $ux \notin E(T)$, $f(r') = -(d_T(x) - d_T(u) + d(N_T[x]) - d(N_T[u]) - \frac{1}{2}r_\Delta - 1 - 1 - 3 - 3 < 4 - 8 = -4$. Thus $f(r') < -4$. Hence T is an l-ancestor of $T(r)$ with respect to f. The argument is reversible to show that if $T(r)$ is an l-ancestor of T with respect to f, then T is an l-descendant of $T(r)$ with respect to f. ■

Now that some sort of order has been established with regards to ancestors and descendants, it is easy to see that a transitivity property immediately follows. We define an l_i-descendant as a descendent generated by a starring triple from R_{l_i}. Let T and T' be trees, and suppose that T' is the l_1-descendant of an l_2-descendant of T. Then we say that T' is an l_1, l_2-descendant of T, and T is an l_2, l_1-ancestor of T'. Suppose that $l_1 = l_2$. Then T' is an l_1^2-descendant of T, and T is an l_1^2-ancestor of T'. We will now demonstrate every tree is a descendant of the path P_n.

Theorem 3. *Let $T \ncong P_n$ be a tree on n vertices. Then*

(i) P_n is an $l_1^{i_1}, l_2^{i_2}, \ldots, l_j^{i_j}$-ancestor of T with respect to g for some $j \geq 1$,

(ii) P_n is an $l_1^{i_1}, l_2^{i_2}, \ldots, l_j^{i_j}$-ancestor of T with respect to f for some $j \geq 1$.

Proof. (i) All we must show is that for any tree $T \ncong P_n$, there exists an l-ancestor T' of T for some $l \geq 1$. Let $v \in S_1(T)$. As $T \ncong P_n$, there is a vertex u such that $d(u) \geq 3$, and let $S = \{u | d(u) \geq 3\}$. Choose $u \in S$ such that $d(v, u) < d(v, u')$ for all $u' \in S - u$, and let P be the v,u-path in T. Additionally, let $y' \in N(u) \cap V(P)$ and $x \in S_1(T) - v$. If $x \in V(P)$, then $S = \emptyset$, a contradiction as $T \ncong P_n$. Thus $r = \{v,u,x\} \in R_l(T)$ where l is the length of P, and $g(r) = d(x) - d(u) \leq 1 - 3 = -2$. Thus $T(r)$ is an l-ancestor of T. Note that $\{u|d_{T(r)}(u) \geq 3\} \leq |S| \leq \{u|d_{T(r)}(u) \geq 3\} + 1$.

(ii) If there exists $u \in S_2(T)$, $d(u) \geq 3$, then consider $r = (v,u,x) \in R_1$, $v,x \in S_1 \cap N(u)$. Then $f(r) = h(r) - \frac{1}{2}r_\Delta = d(N[x]) - d(N[u]) - 1 = (1 + d(u)) - a - 1$ where $a \geq 2d(u)$. Thus $f(r) \leq -d(u) < -2$, and so $T(r)$ is a 1-ancestor of T.

Suppose for all $u \in S_2(T)$, $d(u) = 2$, and let $S = \{s|s \in N(v)$ for some $v \in S_1, d(s) \geq 3\}$. If $S \neq \emptyset$, there exists a $r = (v,u,x) \in R_1$ where $u \in S$ and $x \in S_1 - N(u)$ where $d(N[x]) = 3$. Then $f(r) = h(r) - \frac{1}{2}r_\Delta = d(N[x]) - d(N[u]) - 0 \leq 3 - a - 0$ where $a \geq 2d(u)$. Thus $f(r) \leq -3$, and so $T(r)$ is a 1-ancestor of T.

Suppose $S = \emptyset$. Let $l = \min\{d(u,v)|d(u) = \Delta(T), v \in S_1\}$ where $d(u,v)$ is the distance between u and v, and let v and u be a pair that obtains this minimum length. Let $x \in S_1(T)$. Then choose $r = (v,u,x) \in R_l$. Clearly $r_\Delta = 0$ as $S = \emptyset$, and so $f(r) = g(r) + h(r) - \frac{1}{2}r_\Delta = 1 - d(u) + 3 - a$ where $a \geq 2d(u)$. Then $f(r) \leq -9 < -4$. Thus $T(r)$ is an l-ancestor of T.

Note that in each of these cases, $S_1(T) < S_1(T(r))$, and so P_n is shown to be an $l_1^{i_1}, l_2^{i_2}, \ldots, l_j^{i_j}$-ancestor through a reiteration of this process. ■

Let $j : R \to \mathbb{Z}$ where $j \in \{f,g\}$. It is easy to see that any tree $T \ncong S_n$ has a 1-descendant. Let $r = \{v,u,x\}$ where $\Delta(T) = d(x)$. Then $T(r)$ is an l-descendant of T with respect to j. Thus for any tree T, S_n is an $l_1^{\alpha_1} l_2^{\alpha_2} \ldots l_k^{\alpha_k}$-descendant of T with respect to j. By Theorem 3, we may now construct the sequence of trees that we are seeking.

Definition 4. *Let T be a tree on n vertices and $j \in \{f,g\}$. Then the sequence of trees on n vertices $\{T_i\}_{i=0}^k$ satisfying*

(i) $T_0 \cong P_n$,

(ii) $T_k \cong S_n$,

(iii) $T_{k'} \cong T$ *for some* $0 \leq k' \leq k$,

(iv) T_{i+1} *is an* l_{i+1}*-descendant with respect to* j *of* T_i *for* $0 \leq i \leq k$,

is said to be a genealogy of T with respect to j.

The definition of a genealogy of a tree says that for a given tree, T, there is a sequence of trees starting with P_n and ending with S_n such that T is a member of this sequence. Additionally, given a tree T_i in this sequence, T_{i+1} is an l_{i+1}-descendant for $0 \leq i \leq k-1$. In the subsequent sections, we will show that a genealogy of a tree creates a partial ordering of trees with respect to M_1 and M_2.

3 The First Zagreb Index of a Tree and Its Descendants

A genealogy of a tree extends the works of Das and Gutman and Theorem 1.

Theorem 5. *Let T be a tree and $r \in R_l(T)$. Then $M_1(T(r)) = M_1(T) + 2g(r) + 2$.*

Proof. Let $r = \{v, u, x\} \in R_l(T)$. Then by the definition of $T(r)$, $d_{T(r)}(u) = d_T(u) - 1$, $d_{T(r)}(x) = d_T(x) + 1$, and $d_{T(r)}(z) = d_T(z)$ when $z \neq u, x$.
Consider $M_1(T(r)) - M_1(T)$. Note that

$$\sum_{v \in V((T(r)-\{u,x\})} (d(v))^2 - \sum_{v \in V((T-\{u,x\})} (d(v))^2 = 0$$

Hence,

$$\begin{aligned} M_1(T(r)) - M_1(T) =& (d_T(u) - 1)^2 + (d_T(x) + 1)^2 - ((d_T(u))^2 + (d_T(x))^2) \\ =& 2(d_T(x) - d_T(u)) + 2 \\ =& 2g(r) + 2. \end{aligned}$$

Hence $M_1(T(r)) = M_1(T) + 2g(r) + 2$. ■

By the previous theorem, $M_1(T) < M_1(T(r))$ if $g(r) \geq 0$, $M_1(T) = M_1(T(r))$ if $g(r) = -1$, and $M_1(T) > M_1(T(r))$ if $g(r) \leq -2$. So we have the following corollary.

Corollary 6. *Let $\{T_i\}_{i=0}^k$ be a genealogy of the tree T with respect to g. Then for $T_j, T_{j+1} \in \{T_i\}_{i=0}^k$, $0 \leq j \leq k-1$, $M_1(T_j) \leq M_1(T_{j+1})$.*

Thus for a given tree T, a genealogy of T gives a sequence of trees such that the M_1 value of a tree in the sequence is larger than the M_1 value of any previous tree in this sequence. Hence, a genealogy of T along with M_1 provides a partial ordering of a set of trees on n vertices.

4 The Second Zagreb Index of a Tree and Its Descendants

In a similar way, we will develop a genealogy of a tree T to create a partial ordering of trees with respect to M_2. Let P be the v,u-path of T of length l, $y \in N(u) \cap V(P)$.

Theorem 7. *Let T be a tree and $r \in R_l(T)$. Then*

(i) if $l = 1$

$$M_2(T(r)) = M_2(T) + f(r) + 2.$$

(ii) if $l \geq 2$

$$M_2(T(r)) = M_2(T) + f(r) + 4.$$

Proof. Consider $M_2(T(r)) - M_2(T)$. Note that

$$\sum_{v,z \in V((T(r)) - \{N[u],N[x]\}} d(v)d(z) - \sum_{v,z \in V((T) - \{N[u],N[x]\}} d(v)d(z) = 0$$

Hence when $x \notin N(u)$,

$$\begin{aligned} M_2(T(r)) - M_2(T) &= d(y)d(x) + \sum_{z \in (N_T(x))} d(z) + d(y) - d(y)d(u) - \sum_{z \in (N_T(u)) - y} d(z) \\ &= d(y)(d(x) - d(u)) + (d(N(x) - d(N(u)))) + 2d(y)\ . \end{aligned}$$

When $x \in N(u)$,

$$\begin{aligned} M_2(T(r)) - M_2(T) &= d(y)d(x) + \sum_{z \in (N_T(x))} d(z) - 1 + d(y) - d(y)d(u) - \sum_{z \in (N_T(u)) - y} d(z) \\ &= d(y)(d(x) - d(u)) + (d(N(x) - d(N(u)))) + 2d(y) - 1\ . \end{aligned}$$

Recall when $x \notin N(u)$, $r_\Delta = 0$ and when $x \in N(u)$, $r_\Delta = 2$.

Thus when $l = 1, d(y) = 1$ and $M_2(T(r)) = M_2(T) + f(r) + 2$ and when $l > 2, d(y) = 2$ and $M_2(T(r)) = M_2(T) + f(r) + 4$. ■

By the previous theorem, if $l = 1$, then $M_2(T) < M_2(T(r))$ if $f(r) \geq -1$, $M_2(T) = M_2(T(r))$ if $f(r) = -2$, and $M_2(T) > M_2(T(r))$ if $f(r) \leq -3$. If $l > 1$, then $M_2(T) < M_2(T(r))$ if $f(r) \geq -3$, $M_2(T) = M_2(T(r))$ if $f(r) = -4$, and $M_2(T) > M_2(T(r))$ if $f(r) \leq -5$. So we have the following corollary.

Corollary 8. *Let $\{T_i\}_{i=0}^k$ be a genealogy of the tree T with respect to f. Then for $T_j, T_{j+1} \in \{T_i\}_{i=0}^k$, $0 \leq j \leq k-1$, $M_2(T_j) \leq M_2(T_{j+1})$.*

References

[1] B. Bollobás, P Erdős, Graphs of extremal weights, *Ars. Comb.* **50** (1998) 225–233.

[2] S. Chen, H. Deng, Extremal $(n, n+1)$-graphs with respected to zeroth–order general Randić index, *J. Math. Chem.* **42** (2007) 555–564.

[3] P. Csikvári, On a poset of trees II, *J. Graph Theory* **74** (2013) 81–103.

[4] K. C. Das, Maximizing the sum of the squares of degrees of a graph, *Discr. Math.* **257** (2004) 57–66.

[5] K. C. Das, I. Gutman, Some properties of the second Zagreb index, *MATCH Commun. Math. Comput. Chem.* **52** (2004) 103–112.

[6] D. de Caen, An upper bound on the sum of squares of degrees in a graph, *Discr. Math.* **185** (1998) 245–248.

[7] R. Garcia–Domenech, J. Galvez, J. V. de Julian-Ortiz, L. Pogliani, Some new trends in chemical graph theory, *Chem. Rev.* **108** (2008) 1127–1169.

[8] I. Gutman, K. C. Das, The first Zagreb index 30 years after, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 83–92.

[9] I. Gutman, N. Trinajstić, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* **17** (1972) 535–538.

[10] A. Hou, S. Li, L. Song, B. Wei, Sharp bounds for Zagreb indices of maximal outerplanar graphs, *J. Comb. Optim.* **22** (2011) 252–269.

[11] S. Li, H Zhou, On the maximum and minimum Zagreb indices of graphs with connectivity at most k, *Appl. Math. Lett.* **23** (2010) 128–132.

[12] M. Randić, On characterization of molecular branching, *J. Am. Chem. Soc.* **97** (1975) 6609–6615.