On the maximum and minimum Zagreb indices of some classes of trees

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20th May 2016

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On the extremal Zagreb indices

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- P_n the path, $K_{1,n-1}$ the star

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Theorem (Gutman, Das)

Among *n*-vertex trees, the star $K_{1,n-1}$ has the maximum, and the path P_n has the minimum value of the first (second) Zagreb index. If T_n is an *n*-vertex tree, different from the star or the path, then

$$M_1(P_n) < M_1(T_n) < M_1(K_{1,n-1})$$

and

$$M_2(P_n) < M_1(T_n) < M_2(K_{1,n-1}).$$

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Trees with a given number of maximum degree vertices whose M_1 is minimum

Theorem (B. Borovićanin, T.A. Lampert) Let $T \in \mathcal{T}_{n,k}$, where $1 \le k \le \frac{n}{2} - 1$. Then $M_1(T) \ge 2k + 4n - 6$ (1)

with equality if and only if T has the degree sequence

$$\underbrace{(\underbrace{3,\ldots,3}_{k},\underbrace{2,\ldots,2}_{n-2k-2},\underbrace{1,\ldots,1}_{k+2})}_{(2)}$$

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On the extremal Zagreb indices

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Trees with a given number of maximum degree vertices whose M_1 is maximum

Theorem (B. Borovićanin, T.A. Lampert)
Let
$$T \in \mathcal{T}_{n,k}$$
, where $1 \le k \le \frac{n}{2} - 1$. Then
 $M_1(T) \le k\Delta^2 + p(\Delta - 1)^2 + \mu^2 + n - k - p - 1$, (3)

with equality if and only if T has the degree sequence

$$(\underbrace{\Delta, \dots, \Delta}_{k}, \underbrace{\Delta-1, \dots, \Delta-1}_{p}, \mu, \underbrace{1, \dots, 1}_{n-k-p-1}),$$
(4)
here $\Delta = \lfloor \frac{n-2}{k} \rfloor + 1, p = \lfloor \frac{n-2-k(\Delta-1)}{\Delta-2} \rfloor$ and
 $= n-1-k(\Delta-1)-p(\Delta-2).$

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Theorem (B. Borovićanin, T.A. Lampert) Let $T \in \mathcal{T}_{n,k}$, where $1 \le k \le \frac{n}{2} - 1$. Then

$$M_2(T) \ge \begin{cases} 3k + 4n - 10, & \text{if } n \ge 3k + 1 \\ 6k + 3n - 9, & \text{if } n < 3k + 1. \end{cases}$$

The equality holds if and only if the following three conditions are satisfied.

- (i) The tree *T* has the vertex degree sequence $(\underbrace{3, \ldots, 3}_{k}, \underbrace{2, \ldots, 2}_{n-2k-2}, \underbrace{1, \ldots, 1}_{k+2}).$
- (ii) Between any two vertices of degree 3 in T there should be at least one vertex of degree 2, if possible.
- (iii) The remaining vertices of degree 2 (if they exist) in *T* are placed between two vertices of degree 2, or between a vertex of degree 2 and a vertex of degree 3.

(5)

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 $M_2(T) \le (k-1)\Delta^2 + 2p(\Delta-1)^2 + \mu(\Delta+\mu-1) + \Delta(n-k-(\Delta-1)p-\mu)$, (6)
where $\Delta = \lfloor \frac{n-2}{k} \rfloor + 1$, $p = \lfloor \frac{n-2-k(\Delta-1)}{\Delta-2} \rfloor$ and
 $\mu = n - 1 - k(\Delta - 1) - p(\Delta - 2)$. The equality holds if and only if the
following conditions are satisfied.

(i) The tree
$$T$$
 has the vertex degree sequence $(\Delta, \dots, \Delta, \Delta, \Delta-1, \dots, \Delta-1, \mu, \underbrace{1, \dots, 1}_{n-k-p-1}).$

- (ii) Every vertex of degree $\Delta-1$ is adjacent to a vertex of degree Δ and to $\Delta-2$ pendent vertices.
- (iii) The vertex of degree μ (when $\mu > 1$) is adjacent to a vertex of the degree Δ and to $\mu 1$ pendent vertices.
- (iv) The remaining pendent vertices are attached to the vertices of degree Δ .

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On the maximum Zagreb indices of trees with a given domination number

Theorem (B. Borovićanin, B. Furtula)

Let T be a tree with domination number γ . Then

$$M_1(T) \leqslant (n-\gamma)(n-\gamma+1) + 4(\gamma-1) \tag{7}$$

and

$$M_2(T) \leq 2(n-\gamma+1)(\gamma-1) + (n-\gamma)(n-2\gamma+1). \tag{8}$$

Equality in both cases hold if and only if $T \cong S_{n,n-\gamma}$, where $S_{n,n-\gamma}$ is a spur obtained from the star $K_{1,n-\gamma}$ by attaching a pendent edge to its $\gamma - 1$ pendent vertices.

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• $1 \leqslant \gamma \leqslant n/3$

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- $1 \leqslant \gamma \leqslant n/3$
- $\mathcal{D}(n,\gamma)$ is a set of *n*-vertex trees *T* with domination number γ such that *T* consists of the stars of orders $\lfloor \frac{n-\gamma}{\gamma} \rfloor$ and $\lceil \frac{n-\gamma}{\gamma} \rceil$ with exactly $\gamma 1$ pairs of adjacent leaves in neighboring stars

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Theorem (B. Borovićanin, B. Furtula)

Let T be a tree on n vertices with domination number γ , where $1\leqslant\gamma\leqslant\frac{n}{3}$. Then,

$$M_{1}(T) \geq -\gamma \left\lfloor \frac{n-1}{\gamma} \right\rfloor^{2} + (2n-\gamma) \left\lfloor \frac{n-1}{\gamma} \right\rfloor + 6(\gamma-1).$$
 (9)

The equality holds if and only if $T \in \mathcal{D}(n, \gamma)$.

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- $\frac{n}{3} \leqslant \gamma \leqslant \frac{n}{2}$
- G(n, γ) is a set of trees T on n vertices with domination number γ, such that every vertex from T has at most one pendent neighbor and (i) there exists a minimum dominating set D of T containing 3γ − n − 2 vertices of degree 3 and 2n − 4γ vertices of degree 2, while the set D contains n − 2γ + 2 vertices of degree 2 and 3γ − n pendent vertices, or

(ii) there exists a minimum dominating set D of T containing $n - 2\gamma$ vertices of degree 2 and $3\gamma - n$ pendent vertices, while the set \overline{D} contains $2n - 4\gamma + 2$ vertices of degree 2, $3\gamma - n - 2$ vertices of degree 3 and every vertex from \overline{D} has exactly one neighbor in D.

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Theorem (B. Borovićanin, B. Furtula)

Let T be a tree on n vertices with domination number γ , where $\frac{n}{3}\leqslant\gamma\leqslant\frac{n}{2}$. Then,

$$M_1(T) \geqslant \begin{cases} 4n-6 & \text{if } \gamma = \left\lceil \frac{n}{3} \right\rceil \\ 2n+6\gamma = 10 & \text{if } \frac{n+3}{3} \leqslant \gamma \leqslant \frac{n}{2} \end{cases}$$
(10)

with equality if and only if $T \cong P_n$, for $\gamma = \lceil \frac{n}{3} \rceil$, or $T \in \mathcal{G}(n, \gamma)$, otherwise.

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- A segment of a tree T is a path-subtree S whose terminal vertices are pendent or branching vertices of T, i.e., an internal vertex of a segment S has degree two

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Let S(T) be a tree obtained from T by replacing each segment of T by an edge, it is called *the squeeze* of T

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- M. Goubko, I. Gutman, Degree-based topological indices: Optimal trees with given number of pendents, Appl. Math. Comput. 240 (2014), 387-398.

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• $\mathcal{ST}_{n,k}$ the set of all *n*-vertex trees with exactly *k* segments

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- $\mathcal{ST}_{n,k}$ the set of all *n*-vertex trees with exactly *k* segments
- P_n is the unique element of $ST_{n,1}$; $K_{1,n-1}$ is the unique element of $ST_{n,n-1}$; $ST_{n,2} = \emptyset$

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- $\mathcal{ST}_{n,k}$ for $3 \le k \le n-2$
- A tree is said to be a *starlike of degree k* if it contains exactly one vertex of degree greater than two (the central vertex), and the central vertex has degree k (k ≥ 3)

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The upper bound for M_2 of trees with a given number of sements

Theorem (B. Borovićanin) Let $T \in ST_{n,k}$, where $3 \le k \le n-2$, then

$$M_2(T) \leqslant \begin{cases} 2k^2 - 6k + 4n - 4, & n \ge 2k + 1\\ k(n-3) + 2n - 2, & n < 2k + 1 \end{cases}$$
(11)

The upper bound is attained if and only if T is an *n*-vertex starlike tree of degree k, such that an arbitrary pendent vertex is adjacent to a vertex of degree 2, for $2k + 1 \le n$, or the central vertex of degree k has exactly 2k + 1 - n pendent neighbors, for n < 2k + 1.

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The lower bound for M_2 of trees with a given number of segments

Denote by $ST_O(n, k)$, for odd k, the set of all *n*-vertex trees with the degree sequence

$$\underbrace{(\underbrace{3,\ldots,3}_{\frac{k-1}{2}},\underbrace{2,\ldots,2}_{n-k-1},\underbrace{1,\ldots,1}_{\frac{k+3}{2}})}_{(12)}$$

such that there is at least one vertex of degree 2 between any two vertices of degree 3, and the remaining vertices of degree 2 (if exist) can be placed arbitrarily either between two vertices of degree 2 or between a vertex of degree 2 and a vertex of degree 3.

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The lower bound for M_2 of trees with a given number of segments

Denote by $ST_E(n, k)$, for even k, the set of all *n*-vertex trees with the degree sequence

$$(4, \underbrace{3, \dots, 3}_{\frac{k-4}{2}}, \underbrace{2, \dots, 2}_{n-k-1}, \underbrace{1, \dots, 1}_{\frac{k+4}{2}})$$
(13)

such that the unique vertex of degree 4 has three pendent neighbors and a neighbor of degree 2. The vertices of degree 2 are placed between the vertices of degree 3 (at least one vertex between any two vertices of degree 3, if possible) and the remaining vertices of degree 2 are placed either between two vertices of degree 2 or between the vertex of degree 4 and a vertex of degree 2, or between a vertex of degree 3 and a vertex of degree 2.

The lower bound for M_2 of trees with a given number of segments

Theorem (B. Borovićanin) Let $T \in ST_{n,k}$, where $3 \le k \le n - 2$, then

$$M_{2}(T) \geqslant \begin{cases} \frac{8n+3k-23}{2}, & n \ge \frac{3k-1}{2} \text{ and } k \text{ odd} \\ 3n+3k-12, & n < \frac{3k-1}{2} \text{ and } k \text{ odd} \\ \frac{8n+3k-12}{2}, & n \ge \frac{3k-2}{2} \text{ and } k \text{ even} \\ 3n+3k-10, & n < \frac{3k-2}{2} \text{ and } k \text{ even} \end{cases}$$
(14)

The equality holds if and only if $T \in ST_O(n, k)$, for odd k, or $T \in ST_E(n, k)$, for even k.

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THANK YOU FOR YOUR ATTENTION!

Bojana Borovićanin (PMF Kragujevac)

On the extremal Zagreb indices

20th May 2016 23 / 23

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