Tree with the Extremal Value of Exponential the Forgotten Index

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Abstract

For simple graph G with edge set $E(G)$, $e^{\mathcal{F}_\alpha}(G)=\sum_{uv\in E(G)} e^{d_G^\alpha(u)+d_G^\alpha(v)}$, where $d_G(u)$ is the degree of the vertex u in G, $\alpha\neq 0$ is real. When $\alpha=2$, $e^{\mathcal{F}}(G)=e^{\mathcal{F}_2}(G)$ is called exponential forgotten index of G. In this paper, we first give the extremal value of exponential forgotten index of tree and determine the corresponding extremal graphs. Furthermore, we give the extremal values of exponential index $e^{\mathcal{F}_\alpha}$ of trees, where $\alpha>1$ and determine the corresponding extremal graphs.

Keywords: Tree; Exponential forgotten index; Extremal value; Extremal tree

1 Introduction

In 1972, When study the dependence of π electronic energy structure[1], some chemists found that the energy depends on the square sum of the vertices degrees of the molecular structure(i.e. the first Zagreb index), In fact, the energy is also affected by cubic sum of vertices degree, but this kind of topological index has not been further studied, but forgotten. Therefore, it is called forgotten index, or $\mathcal{F}$ index for short.

Many mathematical chemistry researchers have studied the forgotten index and obtained many good results. For example, B. Furtula, I. Gutman[2] gave a bound on the forgotten index of graphs by using the first Zagreb index and the second Zagreb index; X. Li and H. Zhao [3] discussed the forgotten index of the tree, obtained the extremal value of the tree and characterized the corresponding extremal tree; B. Basavanagoud gave the relationship between the forgotten index of graph and its complement graph. We encourage the reader to consult [5, 6, 7, 8, 9] for the historical background, computational techniques, and mathematical properties of the forgotten index.

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A formal definition of a VDB topological index is as follows. Let $\mathcal{G}_n$ be the set of graphs with n non-isolated vertices. Consider the set

$$K = \{(i,j) \in \mathbf{N} \times \mathbf{N} : 1 \leq i \leq j \leq n-1\}$$

and for a graph $G \in \mathcal{G}_n$, denote by $m_{i,j}(G)$ the number of edges in G joining vertices of degree i and j. A VDB topological index over $\mathcal{G}_n$ is a function $\varphi : \mathcal{G}_n \to \mathbf{R}$ induced by real numbers $\{\varphi_{i,j}\}_{(i,j)\in K}$ defined as

$$\varphi(G) = \sum_{(i,j)\in K} m_{i,j}(G)\varphi_{i,j}$$

for every $G \in \mathcal{G}_n$.

Many important topological indices are obtained from different choices of $\varphi_{i,j}$. For example, the first Zagreb index M_1 induced by numbers $\varphi_{i,j} = i + j$; the second Zagreb index M_2 induced by $\varphi_{i,j} = ij$; the Randić index χ induced by $\varphi_{i,j} = \frac{1}{\sqrt{ij}}$, et al. For details on VDB topological indices, see [10, 11, 12, 13].

Specifically, the forgotten index $\mathcal{F}$ induced by numbers $\varphi_{i,j} = i^2 + j^2$, i.e.

$$\varphi(G) = \sum_{(i,j)\in K} m_{ij}(G)(i^2 + j^2) = \sum_{uv\in E(G)} (d_G^2(u) + d_G^2(v)) = \mathcal{F}(G).$$

In order to study of the discrimination ability of topological indices, Rada [10] introduced the exponential of a vertex-degree-based topological index. Given a vertex-degree-based topological index φ, the exponential of φ, denoted by e^{φ}, is defined as

$$e^{\varphi}(G) = \sum_{(i,j)\in K} m_{i,j}(G)e^{\varphi_{i,j}}$$

So, the exponential forgotten index of G is defined as

$$e^{\mathcal{F}}(G) = \sum_{(i,j)\in K} m_{i,j}(G)e^{i^2+j^2}.$$

For simple graph G,

$$e^{\mathcal{F}_\alpha}(G) = \sum_{(i,j)\in K} m_{i,j}(G)e^{i^\alpha+j^\alpha} = \sum_{uv\in E(G)} e^{d_G^\alpha(u)+d_G^\alpha(v)}.$$

Then, we give the extremal values of exponential index $e^{\mathcal{F}_\alpha}(\alpha > 1)$ of trees and determine the corresponding extremal trees.

2 Trees with maximum exponential forgotten index

Let $\mathcal{T}_n$ is the tree set of all n vertices. We first show in this section that in a maximal tree with respect to $e^{\mathcal{F}}(G)$ over $\mathcal{T}_n$. Furthermore, we find the maximum value of the exponential index $e^{\mathcal{F}_\alpha}(\alpha > 1)$ and the corresponding extremal tree.

Lemma 1. *If T is a maximal tree with respect to $e^{\mathcal{F}}$ in $\mathcal{T}_n$, then the distance between a pendent vertex and a vertex with the maximum degree in T is at most 2.*

Proof Otherwise, there is a vertex u with the maximum degree in T and a path $P = uvw$ such that w is not a pendent vertex in T. Let T_u, T_v and T_w be the components of $T - uv - vw$ containing u, v and w, respectively, see Figure 1. Let $d_T(u) = \Delta$, $d_T(v) = s$, $d(w) = t$, where $\Delta \geq s \geq 2$, $\Delta \geq t \geq 2$. The set of neighbours of v in T is $N_T(v) = \{u, w, v_1, v_2, \cdots, v_{s-2}\}$ with $d_T(v_i) = x_i$ $(i = 1, 2, \cdots, s-2)$, and the set of neighbours of w is $N_T(w) = \{v, w_1, w_2, \cdots, w_{t-1}\}$ with $d(w_j) = y_j$ $(j = 1, 2, \cdots, t-1)$. Let $T' = T - \{ww_1, ww_2, \cdots, ww_{t-1}\} + \{vw_1, vw_2, \cdots, vw_{t-1}\}$, then $d_{T'}(u) = \Delta$, $d_{T'}(v) = s + t - 1$, $d_{T'}(w) = 1$ and

$$
\begin{aligned}
& e^{\mathcal{F}}(T') - e^{\mathcal{F}}(T) \\
&= e^{\Delta^2+(s+t+1)^2} + \sum_{i=1}^{s-2} e^{{x_i}^2+(s+t-1)^2} + \sum_{j=1}^{t-1} e^{{y_j}^2+(s+t-1)^2} + e^{s+t-1^2+1} \\
&- (e^{\Delta^2+s^2} + \sum_{i=1}^{s-2} e^{x_i^2+s^2} + \sum_{j=1}^{t-1} e^{y_j^2+t^2} + e^{s^2+t^2}) \\
&= (e^{\Delta^2+(s+t+1)^2} + e^{s+t-1^2+1} - e^{\Delta^2+s^2} - e^{s^2+t^2}) + \sum_{i=1}^{s-2} (e^{{x_i}^2+(s+t-1)^2} - e^{x_i^2+s^2}) \\
&+ \sum_{j=1}^{t-1} (e^{y_j^2+(s+t-1)^2} - e^{y_j^2+t^2}) + e^{s+t-1} \\
&> e^{\Delta^2+(s+t+1)^2} + e^{s+t-1^2+1} - e^{\Delta^2+s^2} - e^{s^2+t^2} \\
&= e^{s+t-1^2+1}(e^{\Delta^2} + 1) - e^{s^2+t^2}(e^{\Delta^2-t^2} + 1) \\
&> 0,
\end{aligned}
$$

the first greater than is established because $(s+t-1)^2 > s^2$, $(s+t-1)^2 > t^2$, i.e.

$$e^{{x_i}^2+(s+t-1)^2} > e^{x_i^2+s^2}, e^{y_j^2+(s+t-1)^2} > e^{y_j^2+t^2},$$

for $t \geq 2$, $(s+t-1)^2 + 1 > s^2 + t^2$, $\Delta^2 - 1 > \Delta^2 - t^2$, i.e.

$$e^{s+t-1^2+1}(e^{\Delta^2} + 1) - e^{s^2+t^2}(e^{\Delta^2-t^2} + 1) > 0,$$

the second greater than is established.So,

$$e^{\mathcal{F}}(T') > e^{\mathcal{F}}(T).$$

the distance between a pendent vertex and a vertex with the maximum degree in T is at most 2. □

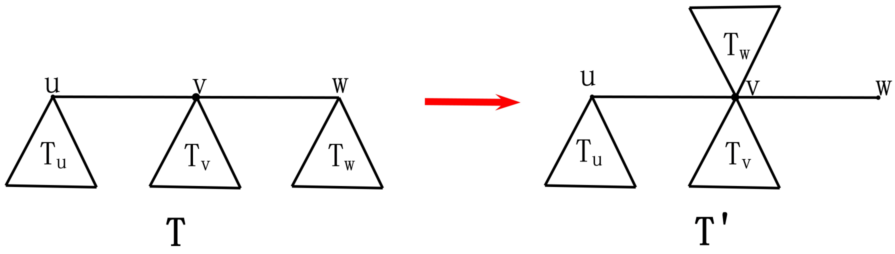

Figure 1. Trees T and T' in Lemma 1

Remark 2. *Let T is a maximal tree with respect to $e^{\mathcal{F}}$ in $T \in \mathcal{T}_n (n \geq 5)$, from Lemma 1, all distances between any pendent vertex and any vertex with the maximum degree are at most 2, then T has the form shown in figure 2, where u is its vertex with the maximum degree.*

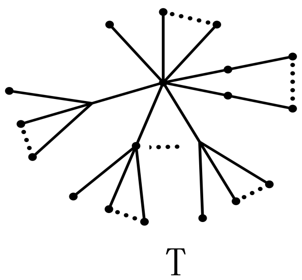

Figure 2. Tree T in remark 2

Theorem 3. *$T \in \mathcal{T}_n (n \geq 5)$, then $e^{\mathcal{F}}(T) \leq (n-1)e^{n^2-2n}$ with equality hold if and only if $T \cong S_n$.*

Proof Let $d_T(u) = \Delta$ be the maximum degree in T. From Lemma 1, if $T \ncong S_n$, then at least one edge uv in T satisfies $d_T(v) = s \geq 2$. If the sets of neighbour of v is $N_T(v)$, then $N_T(v) - \{u\} = \{w_1, w_2, ..., w_{s-1}\} (s \geq 2)$ is leaf in T, the sets of neighbour of u is $N_T(u) = \{v, u_1, u_2, ..., w_{\Delta-1}\}$, where $d_T(u_i) = x_i (i = 1, 2, ..., \Delta - 1)$. Let $T' =$

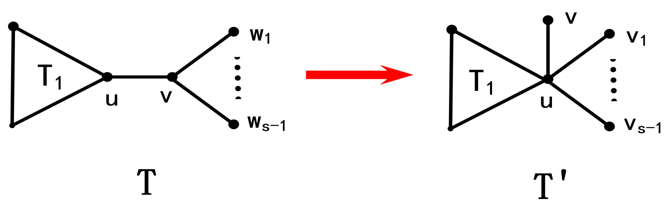

Figure 3. Trees T and T' in theorem 3

$T-\{uw_1, uw_2, ..., u_{s-1}\}+\{vw_1, vw_2, ..., vw_{s-1}\}$, then $d_{T'}(u)=\Delta+s-1$, $d_{T'}(v)=1$, and

$$\begin{aligned}
&e^{\mathcal{F}}(T')-e^{\mathcal{F}}(T)\\
&=(\sum_{i=1}^{\Delta-1} e^{{x_i}^2+(\Delta+s-1)^2}+se^{\Delta+s-1^2+1})-(\sum_{i=1}^{\Delta-1} e^{x_i^2+\Delta^2}+e^{\Delta^2+s^2}+(s-1)e^{s^2+1})\\
&=\sum_{i=1}^{\Delta-1}(e^{{x_i}^2+(\Delta+s-1)^2}-e^{x_i^2+\Delta^2})+(s-1)(e^{\Delta+s-1^2+1}-e^{s^2+1})\\
&+(e^{\Delta+s-1^2+1}-e^{\Delta^2+s^2}),
\end{aligned}$$

obviously, $\Delta+s-1^2>\Delta^2$, $\Delta+s-1^2+1>s^2+1$, $\Delta+s-1^2+1>s^2$, so $e^{\mathcal{F}}(T')-e^{\mathcal{F}}(T)>0$, i.e.

$$e^{\mathcal{F}}(T')>e^{\mathcal{F}}(T).$$

Repeat the above transformation, and from remark 2, we can get the structure of maximal tree $T\approx S_n$. So

$$e^{\mathcal{F}}(T)=e^{\mathcal{F}}(S_n)=(n-1)e^{(n-1)^2}.$$

□

The maximum value problem of exponential forgotten index of tree, i.e. the maximum value problem of $e^{\varphi}(G)(\varphi_{i,j}=i^2+j^2)$ have been solved by above transformation and comparison. In fact, the maximum tree of exponential VDB index $\Sigma_{(i,j)\in K}m_{i,j}(G)e^{(i^\alpha+j^\alpha)}(\alpha\geq 1)$ can also be found through the above methods. Refer to the following corollary.

Corollary 4. *Let $T\in\mathcal{T}_n(n\geq 5)$, if $\varphi_{i,j}=i^\alpha+j^\alpha(\alpha\geq 1)$, then $e^{\varphi}(T)$ get maximum if and only if $T\cong S_n$, and*

$$e^{\varphi}(S_n)=(n-1)e^{(n-1)^\alpha},$$

In particular, when $\alpha=1$, the maximum value of the exponential first Zagreb index in T is $e^{\mathcal{M}_1}(T)=(n-1)e^{n-1}$.

3 Trees with minimum exponential forgotten index

In this section, we mainly use sliding transformation and other methods, consider the minimum value of exponential forgotten index of tree and the corresponding extremal tree, furthermore, we find the minimum value of exponential VDB index e^{φ} and the corresponding extremal tree, where $\varphi_{i,j} = i^{\alpha} + j^{\alpha}$.

Lemma 5. *If T is a minimal tree with respect to $e^{\mathcal{F}}$ in $\mathcal{T}_n (n \geq 5)$, then the maximum degree in T is at most 2.*

Proof $T \in \mathcal{T}_n$, otherwise, there are neighboring vertices u, v in T such that the following conditions: $d_T(u) = s$, $d_T(v) = t > 2$, and a pendent path $P_k = vw_1w_2...w_k$ with length of k, where $w_1 \neq u$, the set of neighbours of v in T is $N_T(v) = \{u, w_1, v_1, v_2, ..., v_{t-2}\}$ with $d_T(v_i) = x_i (i = 1, 2, ..., t-2)$, Let T_u, T_v be the components of $T-uv-vw_1$ containing u, v, respectively, see Figure 4, let $T' = T - \{vv_1, vv_2, ..., vv_{t-2}\} + \{w_kv_1, w_kv_2, ..., w_kv_{t-2}\}$, then $d_{T'}(w_k) = t-1$, $d_{T'}(v) = 2$, if $k = 1$,

$$\begin{aligned}
&e^{\mathcal{F}}(T') - e^{\mathcal{F}}(T) \\
&= (\sum_{i=1}^{t-2} e^{x_i^2+(t-1)^2} + e^{(t-1)^2+2^2} + e^{s^2+2^2}) - (\sum_{i=1}^{t-2} e^{x_i^2+t^2} + e^{t^2+1} + e^{t^2+s^2}) \\
&= \sum_{i=1}^{t-2} (e^{x_i^2+(t-1)^2} - e^{x_i^2+t^2}) + (e^{s^2+4} - e^{s^2+t^2}) + (e^{t^2-2t+5} - e^{t^2+1}).
\end{aligned}$$

$t > 2$, obviously, $x_i^2 + (t-1)^2 < x_i^2 + t^2$, $s^2 + 4 < s^2 + t^2$, $t^2 - 2t + 5 < t^2 + 1$, so $e^{\mathcal{F}}(T') - e^{\mathcal{F}}(T) < 0$. if $k \geq 2$,

$$\begin{aligned}
&e^{\mathcal{F}}(T') - e^{\mathcal{F}}(T) \\
&= (\sum_{i=1}^{t-2} e^{x_i^2+(t-1)^2} + e^{(t-1)^2+2^2} + e^{s^2+2^2} + e^{2^2+2^2}) \\
&- (\sum_{i=1}^{t-2} e^{x_i^2+t^2} + e^{t^2+2^2} + e^{t^2+s^2} + e^{2^2+1^2}) \\
&= \sum_{i=1}^{t-2} (e^{x_i^2+(t-1)^2} - e^{x_i^2+t^2}) + (e^{s^2+4} - e^{s^2+t^2}) \\
&+ (e^{t^2-2t+5} - e^{t^2+4}) + (e^8 - e^5) \\
&\leq (e^{s^2+4} - e^{s^2+t^2}) + (e^{t^2-2t+5} - e^{t^2+4}) + (e^8 - e^5).
\end{aligned}$$

$t > 2$, obviously, $t^2 - 2t + 5 \leq t^2 + 1$, and $s \geq 1$, then

$$(e^{s^2+4} - e^{s^2+t^2}) + (e^8 - e^5) \leq e^{1+4} - e^{1+3^2} + e^8 - e^5 < 0,$$

so $e^{\mathcal{F}}(T') - e^{\mathcal{F}}(T) < 0$.

all above,

$$e^{\mathcal{F}}(T') < e^{\mathcal{F}}(T),$$

contradiction, there are no vertices degree greater than 2. $\square$

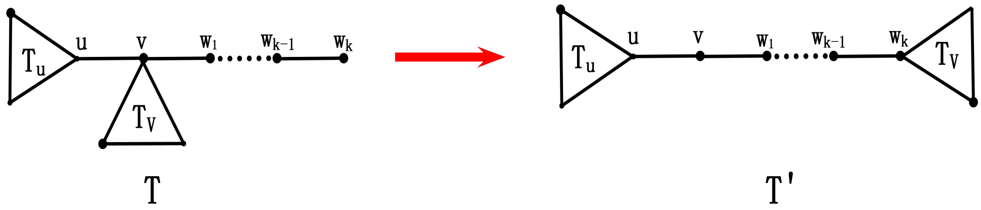

Figure 4. Trees T and T' in Lemma 5

Theorem 6. *Let $T \in \mathcal{T}_n (n \geq 5)$, then $e^{\mathcal{F}}(T) \geq (n-3)e^8 + 2e^5$ with equality hold if and only if $T \cong P_n$.*

Proof From Lemma 5, T is a minimal tree with respect to $e^{\mathcal{F}}$ in $\mathcal{T}_n$, then the maximum degree in T is at most 2. So $T \cong P_n$, i.e.$m_{1,2} = 2,\ \ m_{2,2} = n-3$, and

$$e^{\mathcal{F}}(T) \geq e^{\mathcal{F}}(P_n) = \sum_{(i,j)\in K} m_{i,j}(T)e^{i^2+j^2} = 2e^5 + (n-3)e^8.$$

$\square$

Similar to the problem of tree with minimum value of exponential forgotten index $e^{\mathcal{F}}(T)$, the minimal tree of exponential VDB index $\Sigma_{(i,j)\in K} m_{i,j}(G)e^{(i^\alpha+j^\alpha)} (\alpha \geq 1)$ can also be found through the above methods. Refer to the following corollary.

Corollary 7. *Let $T \in \mathcal{T}_n (n \geq 5)$, $\ \varphi_{i,j} = i^\alpha + j^\alpha (\alpha \geq 1)$, then $e^{\varphi}(T)$ get minimum value if and only if $T \cong P_n$, and*

$$e^{\varphi}(P_n) = 2e^{2^\alpha+1} + (n-3)e^{4^\alpha},$$

In particular, when $\alpha = 1$, the minimum value of the exponential fist Zagreb index in T is $e^{\mathcal{M}_1}(T) = 2e^3 + (n-3)e^4$.

4 Conclusion

Thus, tree with the extremal value of exponential VDB index $e^{\varphi}(G) = \Sigma_{(i,j)\in K} m_{i,j}(G)e^{\varphi_{i,j}}$, where $\varphi_{i,j} = i^\alpha + j^\alpha (\alpha \geq 1)$, have been solved by the above methods. However, we still have no answer to the problem of finding the extremal value of the exponential VDB index $e^{\varphi}(G) = \Sigma_{(i,j)\in K} m_{i,j}(G) e^{\varphi_{i,j}} (\alpha < 1)$ over T_n. Next, we will continue to study this problem.

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