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On Trees with Given Independence Numbers with Maximum Gourava Indices

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Abstract: In mathematical chemistry, molecular descriptors serve an important role, primarily in quantitative structure–property relationship (QSPR) and quantitative structure–activity relationship (QSAR) studies. A topological index of a molecular graph is a real number that is invariant under graph isomorphism conditions and provides information about its size, symmetry, degree of branching, and cyclicity. For any graph N, the first and second Gourava indices are defined as $GO_1(N) = \sum_{u'v' \in E(N)}(d(u') + d(v') + d(u')d(v'))$ and $GO_2(N) = \sum_{u'v' \in E(N)}(d(u') + d(v'))d(u')d(v')$, respectively.The independence number of a graph N, being the cardinality of its maximal independent set, plays a vital role in reading the energies of chemical trees. In this research paper, it is shown that among the family of trees of order δ and independence number ξ, the spur tree denoted as $\Upsilon_{\delta,\xi}$ maximizes both 1st and 2nd Gourava indices, and with these characterizations this graph is unique.

Keywords: tree; spur tree; independence number; Gourava indices

MSC: 05C12; 05C90

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1. Introduction

A topological descriptor is a numerical number assigned to a molecular graph that has applications in quantitative structure–property relationship studies. There are many topological indices available today with applications in chemistry. The structural characteristics of the graphs used to compute the topological indices can be used to characterize them. Let N be a simple graph with the vertex set and edge set denoted by $V(N)$ and $E(N)$, respectively. The degree of a vertex v is denoted by $d(v)$ and is defined as the number of vertices adjacent to v. The neighborhood of vertex v is denoted as $N(v)$ and is the set of vertices adjacent to v. Here, $\Delta(N)$ denotes the maximum degree of the graph. The length of the shortest path between two vertices u and v is known as the distance between them and is denoted as $d(u, v)$. The maximum distance between any two vertices of N is called the diameter of N. If $x' \in V(N)$, $N - x'$ denotes the graph obtained from N by removing x' and its incident edges. Similarly, the graph $N - x'y'$ is a subgraph of N obtained by removing the edge $x'y' \in E(N)$. For a given graph N, a subset W of $V(N)$ is independent if and only if W contains no pairs of adjacent vertices. The independence number of a graph is defined as the cardinality of the maximal independent set and is denoted by $\alpha(N)$. Let $K_{1,n-1}$ and P_n denotethe star and path graphs of order n, respectively. A bipartite graph of order n has at least one partite set, which is also an impartial set, with at least $\frac{n}{2}$ vertices. This indicates that we have $\alpha(T) \geq \lceil \frac{n}{2} \rceil$ for any tree T, and this bound is achieved for the path graph. Additionally, $\alpha(T) \leq n - 1$ and equality holds in case of the star graph. For basic concepts related to graph theory, we refer the readers to [1].

A tree known as a"spur tree" is denoted as $Y_{\delta,\xi}$, where δ and ξ are the order and independence number of the graph, respectively. A spur tree is composed of $\delta - \xi - 1$ paths with a length of 2, each having the same single end vertex and $2\xi - \delta + 1$ pendent vertices attached to that common vertex. Figure 1 shows the spur tree $Y_{\delta,\xi}$. Another definition is that it is obtained by joining a pendent edge to $\delta - \xi - 1$ pendent vertices of $K_{1,\xi}$ with $\alpha(Y_{\delta,\xi}) = \xi$. Das, Xu, and Gutman [2] discovered that the spur tree $Y_{\delta,\xi}$ is the only graph that maximizes both the first and second Zagreb indices in the class of trees with the order δ and independence number ξ. In the same class of trees, Tomescu and Jamil [3] shows that the spur tree $Y_{\delta,\xi}$ is the only graph that maximizes the zeroth-order general Randić index and the general sum-connectivity index $\chi_\alpha(T)$ for $\alpha \geq 1$.

An application of discrete mathematics to chemistry is achieved in 'chemical graph theory', which is applied to study physical and chemical properties of chemical compounds. In chemical graph theory, the molecular structure can be represented using a graph, where the vertices represent the atoms and the edges represent the bond between the atoms. Topological indices are helpful in demonstrating the relationship between the properties of molecules and the chemical structure. Many topological descriptors have been proposed by researchers and used in quantitative structure property relationship studies [4–6]. The first and second Gourava indices [7–9] of a graph N are defined as:

$$GO_1(N) = \sum_{u'v' \in E(N)} (d(u') + d(v') + d(u')d(v')).$$

$$\begin{aligned} GO_2(N) &= \sum_{u'v' \in E(N)} (d(u') + d(v'))d(u')d(v') \\ &= \sum_{u'v' \in E(N)} d(u')^2 d(v') + d(v')^2 d(u'). \end{aligned}$$

Alexander Vasilyev et al. [10] characterized trees with a given order and independence number and with a maximum first Zagreb index. Joyentanuj Das [11] found the maximum value of the Sombor index in the class of trees with a given order and independence number. Mariam et al. [12] provided an upper bound for the first Gourava index of trees with a given order, size, diameter, and pendant vertices. Basavanagoud et al. [13] determined the Gourava and hyper-Gourava indices of cactus chains. For more extremal results related to trees, see [14–19].

The paper is organized as follows. In Section 2, we prove that in the class of trees with a given independence number, the spur tree maximizes the GO_1 index value. In Section 3, it is proven that the spur tree maximizes the GO_2 index values in the class of trees with a given independence number. In Section 4, we give some examples that justify the provided results.

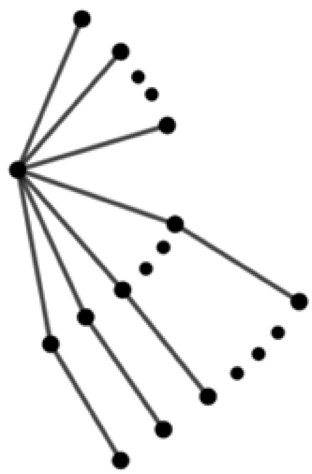

Figure 1. A spur tree.

2. Maximum GO_1 Value of Trees with Given Independence Numbers

Lemma 1. *If $\delta \geq 5$, then the following relation holds:*

$$GO_1\left(\Upsilon_{\delta,\xi}\right) > GO_1(\rho_\delta).$$

Proof. First, we compute $GO_1\left(\Upsilon_{\delta,\xi}\right)$. For this, we need to find the partition of the edges of the spur tree. This partition is depicted in Table 1. Now, using the definition of GO_1, we get:

$$GO_1\left(\Upsilon_{\delta,\xi}\right) = (\xi + 2 + 2\zeta)(\delta - \xi - 1) + (\xi + 1 + \zeta)(2\xi - \delta + 1) + (2 + 1 + 2)(\delta - \xi - 1)$$
$$= \xi^2 + \delta\xi + 6\delta - 6\xi - 6.$$
$$GO_1\left(\Upsilon_{\delta,\xi}\right) = (\xi + 2 + 2\zeta)(\delta - \xi - 1) + (\xi + 1 + \zeta)(2\xi - \delta + 1) + (2 + 1 + 2)(\delta - \xi - 1)$$
$$= \xi^2 + \delta\xi + 6\delta - 6\xi - 6.$$

Additionally:

$$\begin{aligned} GO_1(\rho_\delta) &= 2(1+2+2) + (\delta - 3)(2+2+4) \\ &= 10 + 8\delta - 24 = 8\delta - 14. \end{aligned}$$

Here, we consider:

$$\begin{aligned} GO_1\left(\Upsilon_{\delta,\xi}\right) - GO_1(\rho_\delta) &= \xi^2 + \delta\xi + 6\delta - 6\xi - 6 - (8\delta - 14) \\ &= \xi^2 + \delta\xi - 2\delta - 6\xi + 8. \end{aligned}$$

To prove that $GO_1\left(\Upsilon_{\delta,\xi}\right) > GO_1(\rho_\delta)$, we show that $GO_1\left(\Upsilon_{\delta,\xi}\right) - GO_1(\rho_\delta) > 0$. Let $\delta = 2k'$, then:

$$\begin{aligned} GO_1\left(\Upsilon_{2k',k'}\right) - GO_1(\rho_{2k'}) &= k'^2 + (2k')k' - 2(2k') - 6k' + 8 \\ &= 3k'^2 - 10k' + 8. \end{aligned}$$

Let $\mathcal{F}(x) = 3x^2 - 10x + 8$, then $\mathcal{F}'(x) = 6x - 10 > 0$ for $x \geq 2$. Hence $GO_1\left(\Upsilon_{2k',k'}\right) - GO_1(\rho_{2k'}) > 0$ for $k' > 2$. Now, let $\delta = 2k' + 1$, then:

$$\begin{aligned} GO_1\left(\Upsilon_{2k'+1,k'+1}\right) - GO_1(\rho_{2k'+1}) &= (k'+1)^2 + (2k'+1)(k'+1) - 2(2k'+1) - 6(k'+1) + 8 \\ &= 3k'^2 - 5k' + 8. \end{aligned}$$

Let $\Omega(x) = 3x^2 - 5x + 8$, then $\Omega'(x) = 6x - 5 > 0$ for $x \geq 1$. Hence, $GO_1\left(\Upsilon_{2k'+1,k'+1}\right) - GO_1(\rho_{2k'+1}) > 0$ for $k' > 1$. Thus, we concluded that in both cases we obtained $GO_1\left(\Upsilon_{\delta,\xi}\right) > GO_1(\rho_\delta)$. □

Table 1. The edge partition of $\Upsilon_{\eta,\zeta}$.

Type of Edges	Cardinality of Edges
$(\zeta, 2)$	$\delta - \xi - 1$
$(\zeta, 1)$	$2\xi - \delta + 1$
$(2, 1)$	$\delta - \xi - 1$

Lemma 2. *Let N be a tree and $u \in V(N)$, which is attached to end vertices $v'_1, v'_2, v'_3, \ldots v'_r$. Then, for $r \geq 2$, $v'_1, v'_2, v'_3, \ldots v'_r$ are in any largest independent subset of $V(N)$.*

Theorem 1. *If $\delta \geq 2$, $\frac{\delta}{2} \leq \xi \leq \delta - 1$ and Nisa tree with an order δ and with $\alpha(N) = \xi$, then $GO_1(N)$ is the maximum if and only if $N = \Upsilon_{\delta,\xi}$.*

Proof. We prove the result by applying the principle of mathematical induction on the order of the graph. When the order is 2, we get $\xi = 1$ and $\Upsilon_{2,1} = \rho_2$. When the order is 3, we get $\xi = 2$ and $\Upsilon_{3,2} = \rho_3$. When the order is 4, we get $\xi = 2$, so we get $\Upsilon_{4,2} = \rho_4$, and if $\xi = 3$ we get $\Upsilon_{4,3} = K^*_{1,3}$. These trees are distinct for the particular values of δ and ξ, so the trees have the maximum GO_1 value.Suppose $\delta \geq 5$ and assume that the result holds for all trees with an order $\delta - 1$.

From Lemma 1, we deduce that $GO_1(\rho_\delta)$ cannot be the greatest. Since $\delta \geq 5$, we get $\xi \geq 3$. Assuming the $\xi = 3$, this implies that the order of tree N is equal to 5 or 6. When $\delta = 5$, we get only two trees with $\xi = 3$, given by ρ_5 and $\Upsilon_{5,3}$. When the order is 6 then we get only trees ρ_6 and $\Upsilon_{6,3}$, and the result is verified because ρ_5 and ρ_6 do not have the greatest values of GO_1 (by Lemma 1). As a result, we only consider the situation when $\Delta(N) \geq 3$ and $\xi \geq 4$. Suppose N to be a tree with an order $\delta \geq 5$, with $\Delta(N) \geq 3$ and an independence number $\xi \geq 4$. Let $v'_1, v'_2, v'_3, \ldots, v'_{d+1}$ be the path in N with the greatest length, where d denotes the diameter of N (see Figure 2).We can assume that $d \geq 3$ or else $N = K^*_{1;\delta-1} = \Upsilon_{\delta;\delta-1}$, $\xi = \delta - 1$, and the result is true. Both v'_1 and v'_{d+1} are end vertices.

Now, consider the case when $\alpha(N - v'_1) = \alpha(N)$. If v'_2 is attached to $w' \neq v'_1, v'_3$, then $\hat{d}(w')$ is not greater than 1. Otherwise, the path $v'_1, v'_2, v'_3, \ldots, v'_{d+1}$ in N does not have the greatest length. Therefore, $\hat{d}(w') = 1$, and in lemma 2 both v'_1 and w' are in the greatest independent set. This implies that $\alpha(N - v'_1) = \alpha(N) = 1$ is a contradiction. Thus, $\hat{d}_2 = 2$ and $\hat{d}(v'_3) = v'_3 \leq \Delta(N) \leq \xi$. Keeping in mind the hypothesis of induction, we obtain:

$$
\begin{aligned}
&GO_1(N) - GO_1(N - v'_1) = (1+2+2) + \left(2 + \hat{d}_3\right) + 2\hat{d}_3 - \left(1 + \hat{d}_3\right) + \hat{d}_3 \\
&= 6 + \hat{d}_3 \\
&GO_1(N) = GO_1(N - v'_1) + 6 + \hat{d}_3 \leq GO_1\left(\Upsilon_{\delta-1,\xi}\right) + 6 + \hat{d}_3 \\
&= \xi^2 + \delta\xi + 6\delta - 6\xi - \xi - 6 + \hat{d}_3.
\end{aligned}
$$

The equality holds for $\hat{d}_3 = \xi$ with $GO_1(N) = GO_1\left(\Upsilon_{\delta,\xi}\right)$. Hence, there is equality if and only if $N - v'_1 = \Upsilon_{\delta-1,\xi}$, $\hat{d}(v'_2) = 2$ and $\hat{d}_3 = \xi$, which implies that $N = \Upsilon_{\delta,\xi}$.

Now, we assume the case $\alpha(N - v'_1) = \alpha(N) - 1$. Since the path $v'_1, v'_2, v'_3, \ldots, v'_{d+1}$ (see Figures 3 and 4) in N is of the maximum length with v'_3 in $N(v'_2)$, the only vertex has a degree $\hat{d}_3 \geq 2$. By assuming $\hat{d}(v'_2) = \hat{d}_2 \leq \xi$ and using the induction hypothesis, we obtain:

$$
\begin{aligned}
GO_1(N) - GO_1(N - v'_1) &= \left(1 + \hat{d}_2 + \hat{d}_2\right) + \left(\hat{d}_2 - 2\right)\left(1 + \hat{d}_2 + \hat{d}_2\right) + \left(\hat{d}_2 + \hat{d}_3 + \hat{d}_2\hat{d}_3\right) \\
&\quad - \left(\hat{d}_2 - 2\right)\left(\hat{d}_2 - 1 + 1 + \hat{d}_2 - 1\right) - \left(\hat{d}_2 - 1 + \hat{d}_3 + \left(\hat{d}_2 - 1\right)\hat{d}_3\right) \\
&= \left(1 + 2\hat{d}_2\right)\left(\hat{d}_2 - 1\right) + \hat{d}_3 - 2\hat{d}_2^{\,2} + 5\hat{d}_2 - 1 \\
&= \hat{d}_2 + 2\hat{d}_2^{\,2} - 1 - 2\hat{d}_2 + \hat{d}_3 - 2\hat{d}_2^{\,2} + 5\hat{d}_2 - 1 \\
&= 4\hat{d}_2 + \hat{d}_3 - 2.
\end{aligned}
$$

$$
\begin{aligned}
GO_1(N) &= GO_1(N - v'_1) + 4\hat{d}_2 + \hat{d}_3 - 2 \\
&\leq GO_1\left(\Upsilon_{\delta-1,\xi-1}\right) + 4\hat{d}_2 + \hat{d}_3 - 2 \\
&= (\xi-1)^2 - 6(\xi-1) + 6(\delta-1) + (\delta-1)(\xi-1) - 6 + 4\hat{d}_2 + \hat{d}_3 - 2 \\
&= \xi^2 - 9\xi + 5\delta + \delta\xi - 6 + 4\hat{d}_2 + \hat{d}_3 \\
&= \xi^2 - 9\xi + 5\delta + \delta\xi - 6 + 3\hat{d}_2 + \left(\hat{d}_2 + \hat{d}_3\right).
\end{aligned}
$$

where v'_2 is attached to $\hat{d}_2 - 1$ end vertices. Further, in $N - v'_2v'_3$, we get $\hat{d}(v'_3) = \hat{d}_3 - 1$. Therefore, $\hat{d}_2 - 1 + \hat{d}_3 - 1 \leq \xi$ or $\hat{d}_2 + \hat{d}_3 \leq \xi + 2$. Since at least $\hat{d}_2 + \hat{d}_3 - 2$ end vertices exist in N, we get:

$$
\begin{aligned}
& GO_1(N) = \xi^2 - 9\xi + 5\delta + \delta\xi - 6 + 3\xi + (\xi + 2) \\
& = \xi^2 - 6\xi + 5\delta + \delta\xi + \xi - 4 \\
& = \xi^2 - 6\xi + 5\delta + \delta\xi + \xi - 4 \le GO_1(\Upsilon_\delta, \xi) \\
& = \xi^2 - 6\xi + 5\delta + \delta\xi + \xi - 4 \le \xi^2 + \delta\xi + 6\delta - 6\xi - 6 \\
& 0 \le -6\xi + 5\xi + 6\delta - 5\delta - 6 + 4 \\
& 0 \le \delta - \xi - 2 \\
& \xi \le \delta - 2.
\end{aligned}
$$

$N = K^*_{1,\delta-1} = \Upsilon_{\delta,\delta-1}$, $\xi = \delta - 1$, and the result is true. Hence, we conclude that if $\alpha(N - v'_1) = \alpha(N) - 1$ then we get $GO_1(N) \le GO_1(\Upsilon_{\delta,\xi})$. The only condition for equality is $\xi = \delta - 2$, $N - v'_1 = \Upsilon_{\delta-1,\delta-3}$, $\hat{d}_2 = \xi$, and $\left(\hat{d}_2 + \hat{d}_3\right) = \xi + 2$, such that $\hat{d}_3 = 2$. It follows that there is equality for $N = \Upsilon_{\delta,\delta-2}$ and the theorem is complete. □

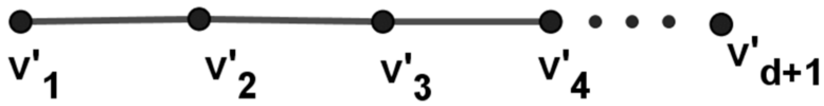

Figure 2. The path of the maximum length in N with degree of $v'_2 = 2$.

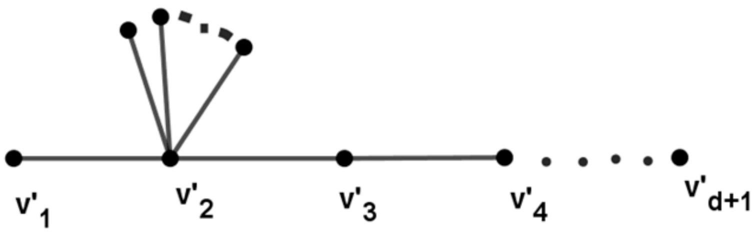

Figure 3. The path of the maximum length in N with degree of v'_2 at least 3.

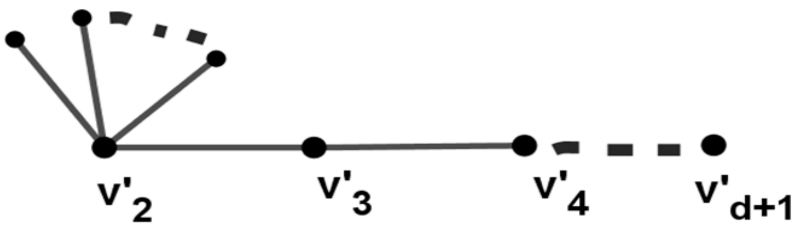

Figure 4. The path of the maximum length with $N - v'_1$.

3. Maximum GO_2 of Trees with Given Independence Number

Lemma 3. *If $\delta \ge 5$, then the following relation holds:*

$$GO_2(\Upsilon_{\delta,\xi}) > GO_2(\rho_\delta).$$

Proof. At first, we compute $GO_2(\Upsilon_{\delta,\xi})$. For this, we need to find the edge partition of the spur tree, which is depicted in Table 1. Now, using the values in the definition of GO_2, we get:

$$
\begin{aligned}
GO_2(\Upsilon_{\delta,\xi}) &= (\xi + 2)(2(\xi)(\delta - \xi - 1) + (\xi + 1)(\xi)(2\xi - \delta + 1) + (2 + 1)(2)(\delta - \xi - 1) \\
&= \delta\xi^2 + 3\delta\xi - 3\xi^2 - 9\xi + 6\delta - 6.
\end{aligned}
$$

Additionally:

$$
\begin{aligned}
GO_2(\rho_\delta) &= 2(1 + 2)2 + (\delta - 3)(2 + 2)4 \\
&= 12 + 16\delta - 48 = 16\delta - 36.
\end{aligned}
$$

Here, we consider:

$$\begin{aligned} GO_2\left(\Upsilon_{\delta,\xi}\right) - GO_2(\rho_\delta) &= \delta\xi^2 + 3\delta\xi - 3\xi^2 - 9\xi + 6\delta - 6 - (16\delta - 36) \\ &= \delta\xi^2 + 3\delta\xi - 3\xi^2 - 9\xi - 10\delta + 30. \end{aligned}$$

To prove that $GO_2\left(\Upsilon_{\delta,\xi}\right) > GO_2(\rho_\delta)$, we show that $GO_2\left(\Upsilon_{\delta,\xi}\right) - GO_2(\rho_\delta) > 0$. For $\delta = 2k'$, we consider:

$$\begin{aligned} GO_2\left(\Upsilon_{2k',k'}\right) - GO_2(\rho_{2k'}) &= (2k')k'^2 + 3(2k')k' - 3k'^2 - 9k' - 10(2k') + 30 \\ &= 2k'^3 + 3k'^2 - 29k' + 30. \end{aligned}$$

Let $\mathcal{F}(x) = 2x^3 + 3x^2 - 29x + 30$, then $\mathcal{F}'(x) = 6x^2 + 6x - 29 > 0$ for $x \geq 2$. This implies that $GO_2\left(\Upsilon_{2k',k'}\right) - GO_2(\rho_{2k'}) > 0$ for $k' > 2$. Now, let $\delta = 2k' + 1$, then consider:

$$\begin{aligned} &GO_2\left(\Upsilon_{2k'+1,k'+1}\right) - GO_2(\rho_{2k'+1}) \\ &= (2k'+1)(k'+1)^2 + 3(2k'+1)(k'+1) - 9(k'+1) - 10(2k'+1) + 30 \\ &= 2k'^3 + 11k'^2 - 16k' + 15. \end{aligned}$$

Let $\Omega(x) = 2x^3 + 11x^2 - 16x + 15$, then $\Omega'(x) = 6x^2 + 22x - 16 > 0$ for $x \geq 1$. This implies that $GO_2\left(\Upsilon_{2k'+1,k'+1}\right) - GO_2(\rho_{2k'+1}) > 0$ for $k' > 1$. Thus, we concluded that in both cases $GO_2\left(\Upsilon_{\delta,\xi}\right) > GO_1(\rho_\delta)$. $\square$

Theorem 2. *If $\delta \geq 2$, $\frac{\delta}{2} \leq \xi \leq \delta - 1$ and N is a tree with an order δ with $\alpha(N) = \xi$, then $GO_2(N)$ is the greatest if and only if $N = \Upsilon_{\delta,\xi}$.*

Proof. We prove the required result by applying the principle of mathematical induction to the order of the graph. When the order is 2, we get $\xi = 1$ and $\Upsilon_{2,1} = \rho_2$. When the order is 3, we get $\xi = 2$ and $\Upsilon_{3,2} = \rho_3$. When the order is 4, we get $\xi = 2$, so if $\Upsilon_{4,2} = \rho_4$ and $\xi = 3$, we get $\Upsilon_{4,3} = K^*_{1,3}$. These trees are distinct for these particular values of δ and ξ, so the trees have the greatest GO_2 index value.

Suppose that $\delta \geq 5$ and assume that the result holds for all trees with an order $\delta - 1$. From lemma 3, we deduce that $GO_2(\rho_\delta)$ cannot be the greatest. Since $\delta \geq 5$, we get $\xi \geq 3$. We assume that $\xi = 3$ implies that the order is 5 or 6. When $\delta = 5$, we get only two trees with $\xi = 3$ given by ρ_5 and $\Upsilon_{5,3}$. When the order is 6, we get only two trees, namely ρ_6 and $\Upsilon_{6,3}$, and the result is verified because ρ_5 and ρ_6 do not have the greatest value for GO_2 (from lemma 3). Therefore, we only consider the situation when $\Delta(N) \geq 3$ and $\xi \geq 4$. Suppose N is a tree with an order $\delta \geq 5$, with $\Delta(N) \geq 3$ and an independence number $\xi \geq 4$. Now, we consider $v'_1, v'_2, v'_3, \ldots, v'_{d+1}$, a path in N of the greatest length, where d denotes the diameter of N (see Figure 1). We can assume that $d \geq 3$ or else $N = K^*_{1,\delta-1} = \Upsilon_{\delta,\delta-1}$, $\xi = \delta - 1$, and the result is true. Both v'_1 and v'_{d+1} are end vertices.

Now, consider the case where $\alpha(N - v'_1) = \alpha(N)$. If v'_2 is attached to $w' \neq v'_1, v'_3$, then $\hat{d}(w')$ is not greater than 1. Otherwise, the path $v'_1, v'_2, v'_3, \ldots, v'_{d+1}$ in N does not have the greatest length; therefore, $\hat{d}(w') = 1$ and from lemma 2 both v'_1 and w' are in the greatest independent set, which implies that $\alpha(N - v'_1) = \alpha(N) - 1$ is a contradiction. Thus, $\hat{d}_2 = 2$ and $\hat{d}(v'_3) = \hat{d}_3 \leq \Delta(N) \leq \xi$. From the induction hypothesis, we get:

$$\begin{aligned} &GO_2(N) - GO_2(N - v'_1) = (1+2)2 + \left(2 + \hat{d}_3\right)2\hat{d}_3 - \left(1 + \hat{d}_3\right)\hat{d}_3 \\ &= 6 + 3\hat{d}_3 + \hat{d}_3{}^2 \\ &GO_2(N) = GO_2(N - v'_1) + 6 + 3\hat{d}_3 + \hat{d}_3{}^2 \\ &\leq GO_2\left(\Upsilon_{\delta-1,\xi}\right) + 6 + 3\hat{d}_3 + \hat{d}_3{}^2 \\ &= \delta\xi^2 - 4\xi^2 + 3\delta\xi - 12\xi + 6\delta + 6 + 3\hat{d}_3 + \hat{d}_3{}^2. \end{aligned}$$

There is equality for $\hat{d}_3 = \xi$, whichimplies that $GO_2(N) = GO_2\left(\Upsilon_{\delta,\xi}\right)$. Hence, for equality, the only conditions are $N - v'_1 = \Upsilon_{\delta-1,\xi}$, $\hat{d}(v'_2) = 2$, and $\hat{d}_3 = \xi$, which imply that $N = \Upsilon_{\delta,\xi}$.

Now, we assume the case of $\alpha(N - v'_1) = \alpha(N) - 1$. Since the path $v'_1, v'_2, v'_3, \ldots, v'_{d+1}$ (see Figures 3 and 4) in N is of the maximum length with v'_3 in $N(v'_2)$, the only vertex has a degree $\hat{d}_3 \geq 2$. Assuming $\hat{d}(v'_2) = \hat{d}_2 \leq \xi$ and using the induction hypothesis, we get:

$$
\begin{aligned}
GO_2(N) - GO_2(N - v'_1) &= \left(1 + \hat{d}_2\right)\hat{d}_2 + \left(\hat{d}_2 - 2\right)\left(\hat{d}_2 + 1\right)\hat{d}_2 + \left(\hat{d}_2 + \hat{d}_3\right)\hat{d}_2\hat{d}_3 \\
&\quad -\left(\hat{d}_2 - 2\right)\left(\hat{d}_2 - 1 + 1\right)\left(\hat{d}_2 - 1\right) - \left(\hat{d}_2 - 1 + \hat{d}_3\right)\left(\hat{d}_2 - 1\right)\hat{d}_3 \\
&= \hat{d}_2 + \hat{d}_2{}^2 + \hat{d}_2{}^3 + \hat{d}_2{}^2 - 2\hat{d}_2{}^2 - 2\hat{d}_2 + \hat{d}_2{}^2\hat{d}_3 + \hat{d}_2\hat{d}_3{}^2 - \hat{d}_2{}^3 \\
&= 3\hat{d}_2{}^2 - 3\hat{d}_2 + \hat{d}_3{}^2 + 2\hat{d}_2\hat{d}_3 - \hat{d}_3 \\
GO_2(N) &= GO_2(N - v'_1) + 3\hat{d}_2{}^2 - 3\hat{d}_2 + \hat{d}_3{}^2 + 2\hat{d}_2\hat{d}_3 - \hat{d}_3 \\
&\leq GO_2\left(\Upsilon_{\delta-1,\xi-1}\right) + 3\hat{d}_2{}^2 - 3\hat{d}_2 + \hat{d}_3{}^2 + 2\hat{d}_2\hat{d}_3 - \hat{d}_3 \\
&= (\delta - 1)(\xi - 1)^2 + 3(\delta - 1)(\xi - 1) - 3(\xi - 1)^2 - 9(\xi - 1) \\
&\quad +6(\delta - 1) - 6 + 3\hat{d}_2{}^2 - 3\hat{d}_2 + \hat{d}_3{}^2 + 2\hat{d}_2\hat{d}_3 - \hat{d}_3.
\end{aligned}
$$

where v'_2 is attached to $\hat{d}_2 - 1$ end vertices and further in $N - v'_2v'_3$ we get $\hat{d}(v'_3) = \hat{d}_3 - 1$. Therefore, $\hat{d}_2 - 1 + \hat{d}_3 - 1 \leq \xi$ or $\hat{d}_2 + \hat{d}_3 \leq \xi + 2$. Since at least $\hat{d}_2 + \hat{d}_3 - 2$ end vertices exist in N, we get:

$$
\begin{aligned}
&GO_2(N) \leq \delta\xi^2 + 4\delta + \delta\xi - 4\xi^2 - 4\xi - 4 + 3\xi^2 - 3\xi + 4 + 4\xi - 2 \\
&= \delta\xi^2 + 4\delta + \delta\xi - \xi^2 - 3\xi - 2 \leq GO_2\left(\Upsilon_{\delta,\xi}\right) \\
&= \delta\xi^2 + 4\delta + \delta\xi - \xi^2 - 3\xi - 2 \leq \delta\xi^2 + 3\delta\xi - 3\xi^2 - 9\xi + 6\delta - 6 \\
&= 4\delta - 6\delta + \delta\xi - 3\delta\xi - \xi^2 + 3\xi^2 - 3\xi + 9\xi - 2 + 6 \leq 0 \\
&= -2\delta - 2\delta\xi + 2\xi^2 + 6\xi + 4 \leq 0 \\
&2\xi^2 + 6\xi + 4 \leq 2\delta + 2\delta\xi \\
&\xi^2 + 3\xi + 2 \leq \delta(\xi + 1) \\
&\xi + 2 \leq \delta \\
&\xi \leq \delta - 2.
\end{aligned}
$$

$N = K^*_{1,\delta-1} = \Upsilon_{\delta,\delta-1}$, $\xi = \delta - 1$, and the result is true. Hence, we conclude that if $\alpha(N - v'_1) = \alpha(N) - 1$, we get $GO_2(N) \leq GO_2\left(\Upsilon_{\delta,\xi}\right)$. The only conditions for equality are $\xi = \delta - 2$, $N - v'_1 = \Upsilon_{\delta-1,\delta-3}$, $\hat{d}_2 = \xi$, and $\hat{d}_2 + \hat{d}_3 = \xi + 2$, such that $\hat{d}_3 = 2$.

It follows that there is equality ξ for $N = \Upsilon_{\delta,\delta-2}$ and the theorem is complete. □

4. Example

For $\delta = 12$ and $\xi = 8$, we verify that for any tree with fixed values of δ and ξ, the theorem is true. First, we compute the 1st and 2nd Gourava indices for $\Upsilon_{\delta,\xi}$:

$$
\begin{aligned}
GO_1\left(\Upsilon_{\delta,\xi}\right) &= \xi^2 + \delta\xi + 6\delta - 6\xi - 6. \\
GO_1(\Upsilon_{12,8}) &= 64 + 96 + 72 - 48 - 6 = 178.
\end{aligned}
$$

$$
\begin{aligned}
GO_2\left(\Upsilon_{\delta,\xi}\right) &= \delta\xi^2 + 3\delta\xi - 3\xi^2 - 9\xi + 6\delta - 6. \\
GO_2(\Upsilon_{12,8}) &= 768 + 288 + 192 - 6 = 858.
\end{aligned}
$$

Now, we compute the 1st and 2nd Gourava indices for trees N'_1, N'_2, and N'_3, as shown in Figure 5.

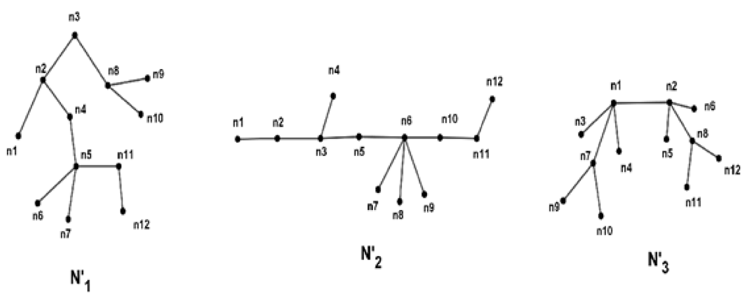

Figure 5. Acyclic structures N'_1, N'_2, N'_3.

$$GO_1(N'_1) = 2(1+4+4) + (1+2+2) + 2(2+4+8) + 3(2+3+6) + 3(1+3+3) = 105.$$

$$GO_2(N'_1) = 2(1+4)4 + (1+2)2 + 2(2+4)8 + 3(2+3)6) + 3(1+3)3 = 268.$$

$$GO_1(N'_2) = 3(1+5+5) + 2(1+2+2) + (2+2+4) + 2(2+5+10) + 2(2+3+6) + (3+1+3) = 114.$$

$$GO_2(N'_2) = 3(1+5)5 + 2(1+2)2 + (2+2)4 + 2(2+5)10 + 2(2+3)6 + (3+1)3 = 330.$$

$$GO_1(N'_3) = 4(1+3+3) + 2(3+4+12) + 4(1+4+4) + (4+4+16) = 126.$$

$$GO_2(N'_3) = 4(1+3)3 + 2(3+4)12 + 4(1+4)4 + (4+4)16 = 552.$$

From Table 2, it is verified that GO_1 and GO_2 are the greatest for $\Upsilon_{12,8}$, which further verifies the results in Theorems 1 and 2.

Table 2. Summary of calculations in example 1 with $\delta = 12$ and $\xi = 8$.

Trees	GO_1	GO_2
$\Upsilon_{12,8}$	178	858
N'_1	105	268
N'_2	114	330
N'_3	126	552

5. Conclusions

In our present discussion, we prove that in the family of trees with an order δ and independence number ξ, the spur tree denoted as $\Upsilon_{\delta,\xi}$ maximizes both the 1st and 2nd Gourava indices, and with these characterizations the graph is unique. In the future, we intend to find maximal graphs of some other classes of graphs, such as bicyclic and tricyclic graphs for different chemical graph invariants.

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