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Research paper

Bicyclic graphs with minimum and maximum forgotten and inverse degree indices

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Abstract

For a connected simple graph G, the inverse degree index and forgotten index are defined as $F(G) = \sum_{uv \in E(G)}[d_u^2 + d_v^2]$ and $ID(G) = \sum_{u \in V(G)} \frac{1}{d_u}$ respectively, where d_u represents the degree of vertex u in G. In this paper, we use some graph transformations and determine the minimum and maximum values of forgotten index and inverse degree index on the class of bicyclic graphs and characterize their corresponding extremal graphs.

1. Introduction

During the last years a large number of topological indices were introduced and found some applications in applied and numerical chemistry [8, 11, 15, 16 and 19]. A topological index is a type of molecular descriptor that is calculated based on the molecular graph of a chemical compound. Topological indices are major invariant to characterize some properties of the graph of a molecule. Several topological indices have been defined and many of them have been found applications as means to model chemical, pharmaceutical and other properties of molecules. Topological indices are generally classified into three kinds: degree-based indices [4, 5, 10], distance-based indices [2] and spectrum-based indices [3]. Topological indices can be used as simple numerical descriptors to compare chemical, physical or biological parameters of molecules in Quantitative Structure Property Relationships (QSPR) and in Quantitative Structure Activity Relationships (QSAR).

All graphs considered in this paper are assumed to be simple and connected. The vertex set and edge set of a graph G are denoted by $V(G)$ and $E(G)$, respectively. The number of neighbors of a vertex u is said to be the degree of u and will be denoted by $d_G(u) = d_u$. A vertex $v \in V(G)$ is said to be pendant, if its neighborhood contains exactly one vertex, i.e. $d_v = 1$. If e is an edge connecting the vertices u and v, then we write $e = uv$. If n is the order of G, then the $n - tuple$ $D = (d_1, d_2, \ldots, d_n)$ of vertex degrees, where $d_i \geq d_{i+1}$ for each $i = 1, 2, \ldots, n$, is called the degree sequence of G. A path P from u_1 to u_i in G is a sequence $P : u_1, e_1, u_2, \ldots, e_{i-1}, u_i$ of alternating vertices and edges such that for every $j = 1, \ldots, i$, e_j is an edge incident with vertices u_j and u_{j+1} and the length of P is $i - 1$. If $u_1 = u_i$, then P is a cycle. A path P is simple, if no vertex occurs twice in P. In addition, P_n and C_n denote the path and the cycle on n vertices, respectively. Let G be a simple graph with p vertices and q edges. If

G has n components, then $\gamma = \gamma(G) = q - p + n$ is called the cyclomatic number of G. A connected graph with $\gamma = 0$ is said to be a tree and graphs with $\gamma = 1, 2$ are called unicyclic and bicyclic, respectively.

The study of topological indices goes back to the seminal work by Wiener [17] in which he used the sum of all shortest path distances nowadays known as the wiener index of a graph. One of the oldest graph invariants is the Zagreb indices first introduced in [9] by Gutman and Trinajstic. For a graph G the inverse degree index was introduced in [6] as

$$ID(G) = \sum_{uv\in E(G)} (\frac{1}{d_u^2} + \frac{1}{d_v^2}) = \sum_{u\in V(G)} \frac{1}{d_u}.$$

In 2006, Zhang [18] introduced the first general Zagreb index of a graph G as follows:

$$M_1^\alpha = M_1^\alpha(G) = \sum_{u\in V(G)} d_u^\alpha.$$

Where α is an arbitrary real number. The forgotten index is just the special case of the first general Zagreb index for $\alpha = 3$. Furtula and Gutman, restudied this index and named it as "forgotten", topological index, or F-index [7]. Thus, F-index is defined as follows:

$$F = F(G) = \sum_{u\in V(G)} d_u^3 = \sum_{uv\in E(G)} (d_u^2 + d_v^2).$$

In 2017, Bozovic et al. [1] used graph transformations and obtained extremal values of total multiplicative sum Zagreb index and first multiplicative sum Zagreb coindex of unicyclic and bicyclic graphs. In [12], we determined extremal values of the inverse degree and the forgotten indices on the class of all unicyclic graphs. In addition, in [13], we found the extremal values of the inverse degree index and forgotten index on the class of unicyclic graphs. In this paper, we use some graph transformations and obtain extremal values of the inverse degree index and forgotten index on the class of all bicyclic graphs.

2. Some graph transformations

Let G be a graph, $V_1 \subseteq V(G)$ and $E_1 \subseteq E(G)$. The subgraph of G obtained by removing the vertices of V_1 and the edges incident with them is denoted by $G - V_1$. Similarly, the subgraph of G obtained by deleting the edges of E_1 is denoted by $G - E_1$. Let $a, b \in V(G)$, $V_1 = \{a\}$ and $E_1 = \{ab\}$. Then the subgraphs $G - V_1$ and $G - E_1$ will be written as $G - a$ and $G - ab$, respectively. In addition, $G \cdot ab$ is a graph, obtained from G by the contraction of edge ab onto vertex a. Finally, if a, b are nonadjacent vertices of G, then $G + ab$ is the graph obtained from G by adding an edge ab.

Theorem 2.1. *Let G and $\widetilde{G}$ be two graphs and $V(G) = V(\widetilde{G}) = V$. Suppose that $u, v \in V(G)$, where $d_G(u) = m$, $d_G(v) = n$, $d_{\widetilde{G}}(u) = m + k$ and $d_{\widetilde{G}}(v) = n - k$, for some $k \geq 0$. If $d_G(a) = d_{\widetilde{G}}(a)$ for each $a \in V \setminus \{u, v\}$, then the following statements hold:*
(i) $k = 0$ or $k = n - m$ if and only if $ID(\widetilde{G}) = ID(G)$,
(ii) $k<n - m$ if and only if $ID(\widetilde{G})<ID(G)$,
(iii) $k>n - m$ if and only if $ID(\widetilde{G})>ID(G)$.

Proof. We set $W = V - \{u, v\}$. Then $d_G(a) = d_{\widetilde{G}}(a)$, for each $a \in W$. Now, by the definition of the inverse degree index, we have

$$\begin{aligned} ID(G) - ID(\widetilde{G}) &= \sum_{a\in V(G)} \frac{1}{d_a} - \sum_{a\in V(\widetilde{G})} \frac{1}{d_a} \\ &= (\frac{1}{d_G(u)} + \frac{1}{d_G(v)}) \\ &\quad -(\frac{1}{d_{\widetilde{G}}(u)} + \frac{1}{d_{\widetilde{G}}(v)}) \\ &= \frac{1}{m} + \frac{1}{n} - (\frac{1}{m+k} + \frac{1}{n-k}) \\ &= \frac{kn^2 - nk^2 - m^2k - mk^2}{mn(m+k)(n-k)} \\ &= \frac{k(n^2 - m^2) - k^2(n+m)}{mn(m+k)(n-k)} \\ &= \frac{k(n+m)(n-m-k)}{mn(m+k)(n-k)}. \end{aligned}$$

Now, it is easy to see that (i), (ii) and (iii)are hold. □

Theorem 2.2. *Let G and $\widetilde{G}$ be two graphs and $V(G) = V(\widetilde{G}) = V$. Suppose that $u, v \in V(G)$, where $d_G(u) = m$, $d_G(v) = n$, $d_{\widetilde{G}}(u) = m + k$ and $d_{\widetilde{G}}(v) = n - k$, for some $k \geq 0$. If $d_G(a) = d_{\widetilde{G}}(a)$ for each $a \in V \setminus \{u, v\}$, then the following statements hold:*
(i) $k = 0$ or $k = n - m$ if and only if $F(\widetilde{G}) = F(G)$,
(ii) $k<n - m$ if and only if $F(\widetilde{G})<F(G)$,
(iii) $k>n - m$ if and only if $F(\widetilde{G})>F(G)$.

Proof. By the same way as in the proof of Theorem 2.1 and the definition of the forgotten index, we have

$$\begin{aligned} F(G)-F(\widetilde{G}) &= \sum_{a\in V(G)} d_a^3 - \sum_{a\in V(\widetilde{G})} d_a^3 \\ &= (d_G^3(u)+d_G^3(v)) \\ &\quad -[(d_{\widetilde{G}}^3(u)+d_{\widetilde{G}}^3(v)] \\ &= m^3+n^3-(m+k)^3-(n-k)^3 \\ &= 3n^2k-3m^2k-3nk^2-3mk^2 \\ &= 3k(n^2-m^2)-3k^2(m+n) \\ &= 3k(m+n)(n-m-k). \end{aligned}$$

Now, we can see that (i), (ii) and (iii) are hold. □

A graph transfformation converts the information from the primary graph into a new converted structure. Now, we present several well-known graph transformations [1, 14] that will be used to attain our main results.

Pendant-Path (PP) Transformation. Let G be a nontrivial graph, $u, v \in V(G)$ and $d_G(v) \geq 3$. Suppose that $P_1 : uu_1u_2\dots u_s$ and $P_2 : vv_1v_2\dots v_t$ are two paths, that hang on u and v, respectively. Let $\widetilde{G}$ be the graph achieved from G by interconnecting P_1 and P_2 (see Fig. 1). Therefore, the $uu_1...u_sv_1...v_t$ is a path in the new graph $\widetilde{G}$.

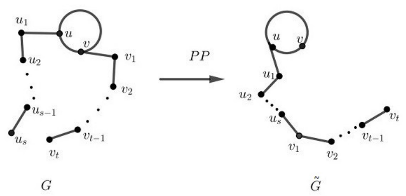

Figure 1. PP Transformation

If we use PP transformation on G, then the degree of u_s increases by $k = 1$ and the degree of v decreases by $k = 1$. Also, the degrees of other vertices in G and $\widetilde{G}$ are equal. Therefore, Theorem 2.1 and Theorem 2.2 show that $ID(\widetilde{G}) < ID(G)$ and $F(\widetilde{G}) < F(G)$.

Contraction to path (EP) Transformation. Let G be a nontrivial graph. Consider two adjacent vertices u and v in G and let $d_G(u) \geq 3$ and $P : uu_1u_2\dots u_s$ be a path in G. We remove the edge uv and add the new edge u_sv. We denote the new obtained graph by $\widetilde{G}$ (see Fig. 2).

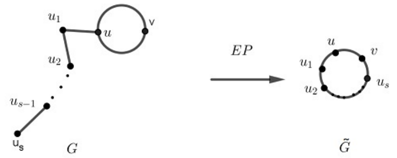

Figure 2. EP Transformation

Let $d_G(u_s) = m$, $d_G(u) = n$ and $n \geq 3$. If we use EP transformation on G, then $d_{\widetilde{G}}(u_s) = m+1$, $d_{\widetilde{G}}(u) = n-1$, and the degrees of other vertices in G and $\widetilde{G}$ are the same. Now by Theorem 2.1 and Theorem 2.2, $ID(\widetilde{G}) < ID(G)$ and $F(\widetilde{G}) < F(G)$.

Contraction to star (CS) Transformation. Suppose that G is a graph, $u, v \in V(G)$ and u and v have no shared neighbor. Let $d_G(u) = m$ and $d_G(v) = n$, where $m \geq n \geq 2$. If $e = uv$, we show $(G.e) + uv$ by $\widetilde{G}$ (Fi. 4).

Let u and v be two vertices of a graph G with $d_G(u) = m$ and $d_G(v) = n$. If we use CS transformation on G, then $d_{\widetilde{G}}(v) = n-(n-1) = 1$ and $d_{\widetilde{G}}(u) = m+(n-1)$ and the degrees of other vertices in G and $\widetilde{G}$ are equal. By Theorem 2.1 and Theorem 2.2, if $m \geq n \geq 2$, then $ID(\widetilde{G}) > ID(G)$ and $F(\widetilde{G}) > F(G)$.

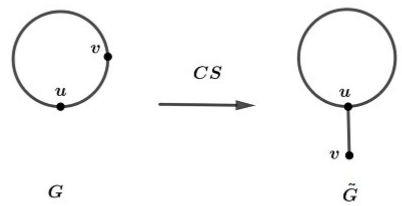

Figure 3. CS Transformation

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Star translation (ST) Transformation. Let G be a graph, $v \in V(G)$ and $v_1, v_2, \dots, v_t$ be pendant vertices and neighbors of vertex v. If $u \in V(G) - \{v_1, v_2, \dots, v_t\}$, then we show $(G - \{vv_1, vv_2, \dots, vv_t\}) + \{uv_1, uv_2, \dots, uv_t\}$ by $\widetilde{G}$ (Fig. 4). Now, if $d_G(u) = m$ and $d_G(v) = n$, then by Theorem 2.1 and Theorem 2.2 we have

(a) If $t = n - m$, then $ID(\widetilde{G}) = ID(G)$ and $F(\widetilde{G}) = F(G)$,

(b) If $n - m > t$ and $t>0$, then $ID(\widetilde{G}) < ID(G)$ and $F(\widetilde{G}) < F(G)$,

(c) If $t > n - m$, then $ID(\widetilde{G}) > ID(G)$ and $F(\widetilde{G}) > F(G)$.

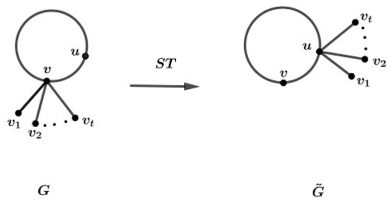

Figure 4. ST Transformation

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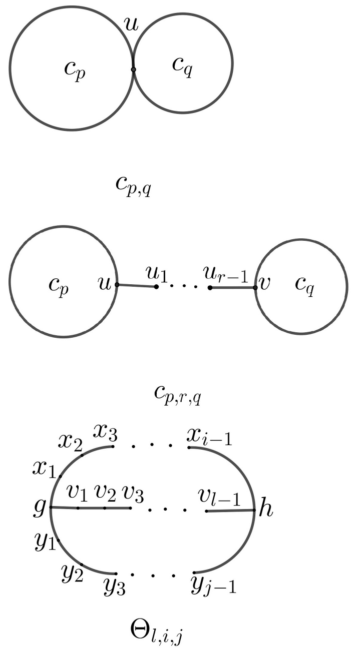

Figure 5. Main subgraphs of bicyclic graphs

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3. Maximal and minimal values of inverse degree and forgotten indices on bicyclic graphs

In this section, we achieve extremal graphs with respect to the inverse degree and the forgotten indices on the class of all bicyclic graphs, by considering the main subgraphs of the bicyclic graphs.

If G is a bicyclic graph, then G possesses two independent cycles and these cycles are denoted by C_p and C_q as in [16]. Now, one of the following cases will be occurred:

(I) The subgraph C_p and C_q in graph G possess exactly one shared vertex u.

(II) The subgraph C_p and C_q in graph G are connected by a path of length r, where $r>0$.

(III) The subgraph C_{l+i} and C_{l+j} in G, posses a shared path of length l, where $0 < l \leq min\{i, j\}$.

The subgraphs $C_{p,q}$, $C_{p,r,q}$ and $\Theta_{l,i,j}$, depending on the previous three cases, are called main subgraphs of G, respectively (see Fig. 5).

If G is a bicyclic graph, we transform each tree of G into a path by frequentative use of PP transformation. Then, we transform all the paths with the same transformation into a unique path such as $P : w_1w_2 \dots w_t$. Thereupon, we acquire a bicyclic graph $\widetilde{G}$ such that the main subgraph of $\widetilde{G}$ is one of the graphs $C_{p,q}$, $C_{p,r,q}$ or $\Theta_{l,i,j}$ and it has a unique pendent path P attached at one of its vertices. According to the main subgraph of $\widetilde{G}$, we consider the following three cases:

$Case\ A$: **The main subgraph of $\widetilde{G}$ is $C_{p,q}$**

If the path P was connected to the vertex u, then we displace P and paste it to a vertex in C_p or C_q except u. Thus, we assume that P is attached to the vertex s, where $s \neq u$. Now, if the EP transformation is used for s and one of its neighbors of degree 2, we obtain a graph of type I, where the length of one of its cycles is increased by the length of P as Fig. 6. Also, we show that EP transformation decreases the inverse degree and the forgotten indices.

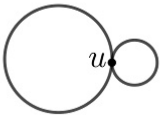

Figure 6. Bicyclic graph φ_1 of type I

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$Case\ B$: **The main subgraph of $\widetilde{G}$ is $C_{p,r,q}$**

If the path P was connected to the vertices $\{u, u_1, u_2, \ldots, u_{r-1}, v\}$, then we displace and paste it to a vertex s in C_p or C_q except u and v. Now, if the EP transformation is used for s and one of its neighbors of degree 2, then we obtain a graph of type II, where the length of one of its cycles is increased by the length of P. In addition, the vertices $\{u_1, u_2, \ldots, u_{r-1}\}$ can be inserted into one of the cycles C_p or C_q. In this way, the degree sequence of the graph does not change, so the inverse degree and the forgotten indices do not change. Eventually, we achieve a bicyclic graph, where its cycles are linked by uv as in the Fig. 7.

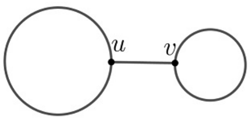

Figure 7. Bicyclic graph φ_2 of type II

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$Case\ C$: **The main subgraph of $\widetilde{G}$ is $\Theta_{l,i,j}$**

Similar to the previous cases, if the path P was connected to one of the vertices $\{g, v_1, v_2, \ldots, v_{l-1}, h\}$, then we displace and paste it to a vertex s in C_p or C_q except g and h. Now, if the EP transformation is used for s and one of its neighbors of degree 2, then we obtain a graph of type III, where the length of one of its cycles is increased by the length of P. In addition, the vertices $\{v_1, v_2, \ldots, v_{l-1}\}$ can be inserted into one of the cycles C_p or C_q. In this way, the degree sequence of the graph does not change, so the inverse degree and the forgotten indices do not change. Eventually, we achieve a bicyclic graph of type III, where its cycles are shared in the edge gh as Fig. 8.

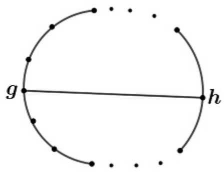

Figure 8. Bicyclic graph φ_3 of type III

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Therefore, every bicyclic graph G can be converted into one of the graphs φ_1 (Fig. 6), φ_2 (Fig. 7) or φ_3 (Fig. 8). The degree sequences of φ_2 and φ_3 are the same. In the next lemma, we compare the inverse degree and the forgotten indices of φ_1 and φ_2.

Lemma 3.1. *Let φ_1, φ_2 and φ_3 be the simple bicyclic graphs Fig. 6, Fig. 7 and Fig. 8, respectively. Then*
$(a)\ ID(\varphi_1) > ID(\varphi_2) = ID(\varphi_3),$
$(b)\ F(\varphi_1) > F(\varphi_2) = F(\varphi_3).$

Proof. (a) We can see that the degree sequence of φ_1 is (4,2,2,...,2) and φ_2 is (3,3,2,2,...,2). Then by the definition we have

$$\begin{aligned} ID(\varphi_1) - ID(\varphi_2) &= \sum_{u \in V(G)} \frac{1}{\acute{d}_u} - \sum_{u \in V(G)} \frac{1}{d_u} \\ &= (\frac{1}{2} + \ldots + \frac{1}{2} + \frac{1}{4}) \\ &\quad -(\frac{1}{2} + \ldots + \frac{1}{2} + \frac{1}{3} + \frac{1}{3}) \\ &= \frac{1}{12}. \end{aligned}$$

Thus, $ID(\varphi_1) - ID(\varphi_2) > 0$ and $ID(\varphi_2) < ID(\varphi_1)$, for each $n \geq 5$.

(b)With a similar argument for the forgotten index , we have

$$\begin{aligned} F(\varphi_1) - F(\varphi_2) &= \sum_{u \in V(G)} \acute{d}_u^3 - \sum_{u \in V(G)} d_u^3 \\ &= (2^3 + \ldots + 2^3 + 4^3) \\ &\quad -(2^3 + \ldots + 2^3 + 3^3 + 3^3) \\ &= 18. \end{aligned}$$

Therefore, $F(\varphi_1) - F(\varphi_2) > 0$ and $F(\varphi_2) < F(\varphi_1)$, for each n $n \geq 5$. $\square$

If G is a bicyclic graph, then by iterative use of the CS transformation, G can be converted to a bicyclic graph $\widetilde{G}$, where $\widetilde{G}$ consists of two triangles and some hanging stars and the inverse degree index of $\widetilde{G}$ is greater than the inverse degree index of G and its forgotten index is greater than the forgotten index of G. Now, we repeat ST transformation until G converts to ψ_1 or ψ_2 of Fig. 9. Also, ST transformation increases the inverse degree and the forgotten indices.

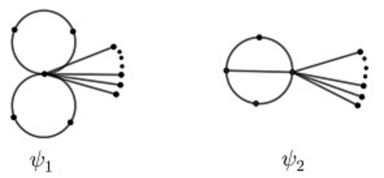

Figure 9. Bicyclic graphs ψ_1 and ψ_2

In the next lemma, we compare the inverse degree and forgotten indices of the graphs ψ_1 and ψ_2.

Lemma 3.2. *Let ψ_1 and ψ_2 be the simple bicyclic graphs Fig. 9. Then*
(a) $ID(\psi_1) < ID(\psi_2)$,
(b) $F(\psi_1) < F(\psi_2)$.

Proof. (a) We can see that the degree sequence of ψ_1 is (n-1,2,2,2,2,1,1,...,1) and ψ_2 is (n-1,3,2,2,1,1,...,1), so by the definition we have

$$ID(\psi_1) - ID(\psi_2) = \sum_{u\in V(G)} \frac{1}{\acute{d}_u} - \sum_{u\in V(G)} \frac{1}{d_u}$$
$$= \left(\frac{1}{1} + \ldots + \frac{1}{1} + \frac{1}{2} + \frac{1}{2} + \frac{1}{2} + \frac{1}{2} + \frac{1}{n-1}\right)$$
$$- \left(\frac{1}{1} + \ldots + \frac{1}{1} + \frac{1}{2} + \frac{1}{2} + \frac{1}{3} + \frac{1}{n-1}\right)$$
$$= \frac{-1}{3}.$$

Thus, $ID(\psi_1) - ID(\psi_2) < 0$ and $ID(\psi_1) < ID(\psi_2)$, for each $n \geq 5$.

(b)With a Similar argument above for forgotten index, we have

$$F(\psi_1) - F(\psi_2) = \sum_{u\in V(G)} \acute{d}_u^3 - \sum_{u\in V(G)} d_u^3$$
$$= 1^3 + \ldots + 1^3 + 2^3 + 2^3 + 2^3 + 2^3 + (n-1)^3$$
$$-(1^3 + \ldots + 1^3 + 2^3 + 2^3 + 3^3 + (n-1)^3)$$
$$= -12.$$

Therefore, $F(\psi_1) - F(\psi_2) < 0$ and $F(\psi_1) < F(\psi_2)$, for each $n \geq 5$. □

Now, by the above explanations we can prove the main results of this section.

Theorem 3.3. *Let G be a bicyclic graphs of order n, where $n \geq 5$. Then*
(i) $ID(\varphi_2) \leq ID(G) \leq ID(\psi_2)$,
(ii) $F(\varphi_2) \leq F(G) \leq F(\psi_2)$.

Proof. (i) If G is a bicyclic graph, then we show that G can be converted into one of the graphs φ_1, φ_2 or φ_3 of Lemma 3.1, by the PP and EP transformations and these transformations decrease the inverse degree index. Therefore, Lemma 3.1 implies that $ID(\varphi_2) \leq ID(G)$. Similarly, G can be converted into one of the graphs ψ_1 or ψ_2 of Lemma 3.2 by the CS and ST transformations and these transformations increase the inverse degree index. Therefore, Lemma 3.2 shows that $ID(G) \leq ID(\psi_2)$.

Another part can be proved by a similar argument. □

4. Conclusion

In this article, we used some well known graph transformations to obtain the extremal graphs with respect to the forgotten index and the inverse degree index on the class of all bicyclic graphs. We showed that, if G is a bicyclic graph of order n, where $n \geq 5$, then $\frac{n-2}{2} + \frac{2}{3} \leq ID(G) \leq \frac{n^2-5n+5}{n-1} + \frac{4}{3}$ and $8n + 38 \leq F(G) \leq n^3 - 3n^2 + 4n + 42$.

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