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BOUNDS FOR THE SUM OF CUBES OF VERTEX DEGREES OF SPLICE GRAPHS

VEEREBRADIAH LOKESHA[1], SUSHMITHA JAIN[1], MANJUNATH MUDDALAPURAM [1],
AHMET SINAN CEVIK[2], ISMAIL NACI CANGUL[3], §

Abstract. Some chemically interesting graphs can be derived from simpler graphs by some graph operations. One of the most relevant among these interesting graphs is named as splice graphs. They are related to RNA sequencing and therefore is of great interest. The main target of this paper is to obtain the explicit interpretation of F-index in terms of the graph size and maximum or minimum vertex degrees of special splice graphs.

Keywords and Phrases: F-index, forgotten index, splice graph, RNA sequence.

Mathematics Subject Classification: 05C05, 05C12

1. Introduction

A graphical invariant is a number obtained corresponding to a graph or equivalently, it is a fixed number under graph automorphisms. That is, for isomorphic graphs, it has the same value. In chemical graph theory, these invariants are also called the topological indices. Topological indices play a crucial part in mathematical chemistry, especially in QSAR/QSPR investigations, see [19] for the details. Wiener index, Zagreb indices, forgotten index, symmetric division degree index are some of those frequently studied invariants.

The first and second Zagreb indices of a graph G, defined by $M_1(G) = \sum_{u\in V(G)} d(u)^2$ and $M_2(G) = \sum_{uv\in E(G)}[d(u)d(v)]$, respectively, are the oldest, most popular and extremely studied vertex degree based topological indices (we may refer to, for instance,

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[1] Department of Studies in Mathematics VSK University, Bellary, Karnataka, India.
e-mail: lokiv@yahoo.com; ORCID: https://orcid.org/0000-0003-2468-9511.
e-mail: sushmithajain9@gmail.com; ORCID: https://orcid.org/0000-0002-4173-8787.
e-mail: manju3479@gmail.com; ORCID: https://orcid.org/0000-0003-1328-6215.
[2] Department of Mathematics, Science Faculty, King Abdulaziz University, 21589, Jeddah, Saudi Arabia.
Department of Mathematics, Faculty of Science, Selcuk University, Konya, 42130, Turkey.
e-mail: ahmetsinancevik@gmail.com; ORCID: https://orcid.org/0000-0002-7539-5065.
[3] Department of Mathematics, Faculty of Arts and Science, Bursa Uludag University, 16059, Bursa, Turkey.
e-mail: cangul@uludag.edu.tr; ORCID: https://orcid.org/0000-0002-0700-5774; corresponding author.
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[7, 10, 15, 20, 22, 33]). Although these indices were introduced to study the structure-dependency of the total π-electron energy, see [14], in the same study, one more topological index was defined as the sum of cubes of degrees of the vertices of a given graph G as follows:

$$F(G) = \sum_{u \in V(G)} d(u)^3. \tag{1}$$

But this index was no further studied till a paper written by Furtula and Gutman, [11]. In fact the authors concluded that the predictive ability of this index is almost near to that of the first Zagreb index and, for the entropy and acentric factor, both of them yield correlation coefficients greater than 0.954. They termed this index given in Eqn. (1) as *forgotten topological index* or shortly *F-index*.

Some chemically interesting graphs are obtained by means of different graph operations which can be thought as graph extensions on some general or particular graphs, [1, 4, 13, 21, 31]. The reason for studying these operations is to understand how the graph operation can relate the values of the corresponding topological indices of the given graphs to the values of the topological indices of the larger graph obtained as a result of this operation or sometimes to the help us to comment on chemical properties of the component graphs or the resulting graph. Actually this idea has similarities, for instance, to group extensions in pure algebra. In the next paragraph we will remind one of the graph operations, namely splice graphs and they will be the main graph type that we shall be considering throughout this paper.

Let G and H be two simple connected graphs with disjoint vertex sets $V(G)$ and $V(H)$, and edge sets $E(G)$ and $E(H)$, respectively. Let $a_1 \in V(G)$ and $x_1 \in V(H)$. Then the *splice graph* $\mathcal{S} = \mathcal{S}(G, H)$ of G and H by vertices a_1 and x_1, respectively, is defined by identifying the vertices a_1 and x_1 in the union of G and H (see, for instance, [9, 2, 29]). It is known that, for splice graphs, the total number of vertices is $n_G + n_H - 1$ while the total number of edges is $e_G + e_H$.

Long non-coding RNAs (lncRNAs), a type of transcripts that are longer than 200 nucleotides and unable to encode proteins in the intracellular space, have been at the forefront in recent years. Several studies indicate that more than 80 percent of the human genome has biochemical functions. These figures suggest that lncRNAs hide lots of valuable information which are waiting to be discovered. Only a small amount of lncRNAs have already been studied, but scientists have discovered some biological processes such as epigenetic regulation, metabolic processes, chromosome dynamics and cell differentiation, [3, 25]. Lots of evidence have indicated that lncRNAs are highly relevant to various complex human diseases, [5], such as lung cancer, [30], Alzheimer diseases, [24], and cardiovascular diseases, [6].

Sequencing studies on some organisms often interrogate both genomes and transcriptomes with massive amounts of short sequences. Such studies require de novo analysis tools and techniques, when the species and closely related species lack high quality reference resources. For certain applications such as de novo annotation, information on putative exons and alternative splicing may be desirable.

In [18], a new method called ChopStitch for finding putative exons de novo and constructing splice graphs using an assembled transcriptome and hence whole genome sequencing data have been constructed. ChopStitch identifies exon-exon boundaries in de novo assembled RNA-Seq data with the help of a filter. The primary output of the tool is a file containing putative exons. Further, exon edges are interrogated for alternative exon-exon boundaries to detect transcript isoforms, which are naturally represented as splice graphs.

After constructing the genomic filter, ChopStitch searches for the transcript sequences to find putative exons. It then finds exons with overlapping edges and constructs a splice-graph. A program Graphviz ccomps is used to find subgraphs which also give several properties of some parts of the sequence under investigation. Therefore, new studies discovering mathematical properties of splice graphs will help to discover physicochemical properties of DNA and RNA sequences, and surely have a lot of applications. This is our main motivation for this study.

Now let us recall two special graphs which will be needed in our main construction and in the proofs of the results of this paper. First of all, the subdivision graph $S(G)$ of G is the graph obtained by inserting an additional vertex to each edge of G, in other words, by replacing each edge of G by a path of length 2, [23, 26, 27]. Secondly, $R(G)$ is the graph derived from G by adding a new vertex not on any edge of G corresponding to each edge of G and by connecting this new vertex to both vertices of the corresponding edge, see for instance, [28].

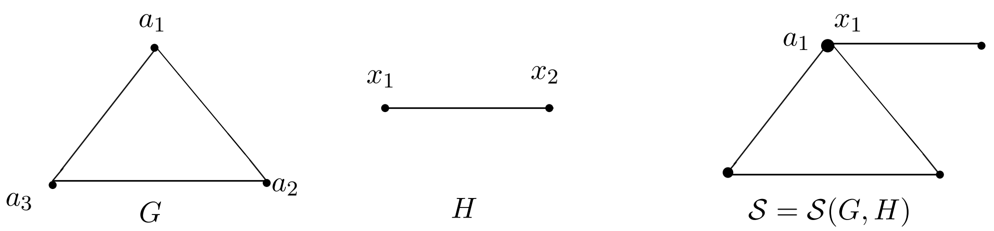

FIGURE 1. A splice of G and H by vertices a_1 and x_1

In [8], De presented several types of corona products of these two derived graph types. Motivated by this study and by [29], in this paper, we will first introduce different types of splice graphs such as R-vertex and S-vertex splice, R-edge and S-edge splice, R-vertex neighborhood and S-vertex neighborhood splice, R-edge neighborhood and S-edge neighborhood splice, and then we will give the explicit expressions of F-index for these new kinds of splice graphs.

2. Main results

Our results will be given in different subsections by presenting the related definition at first. For a graph G, we let Δ_G and δ_G represent the maximum and minimum vertex degrees, respectively, and let n_G and e_G denote the number of vertices and edges as usual.

2.1. **S-vertex and R-vertex splice.** In this section, we first introduce S-vertex and R-vertex splices. Let G and H be two vertex disjoint graphs. Let $a_1 \in V(G)$ and $x_1 \in V(H)$.

Definition 2.1. *The S-vertex splice $\mathcal{S}_v$ (or the R-vertex splice $\mathcal{S}_{vR}$) of G and H is obtained from $S(G)$ (or from $R(G)$) and one copy of H by identifying the vertices a_1 and x_1 in the union of $S(G)$ (or $R(G)$) and H.*

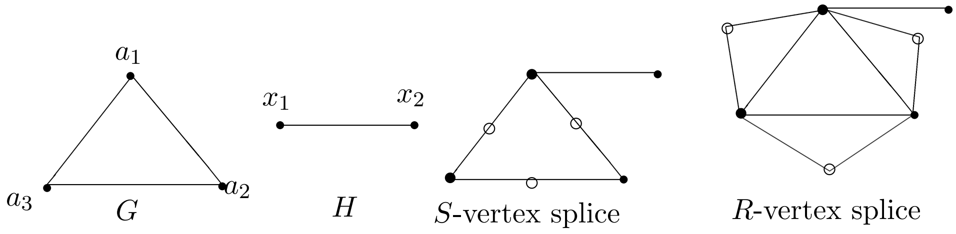

FIGURE 2. S- and R-vertex splices

In the following results, some upper and lower bounds for the F-index of S-vertex and R-vertex splice graphs are given:

Theorem 2.1. *A lower and an upper bound for the F-index of the S-vertex splice graph $\mathcal{S}_v$ are given by*

$$F(\mathcal{S}_v) \quad \leq F(G) + F(H) + 8e_G + 3\Delta_G\Delta_H\big(\Delta_G + \Delta_H\big)$$

and

$$F(\mathcal{S}_v) \quad \geq F(G) + F(H) + 8e_G + 3\delta_G\delta_H\big(\delta_G + \delta_H\big).$$

Proof. By Eqn. (1), we can write

$$F(\mathcal{S}_v) \quad = \quad \sum_{i=1}^{n_G-1}(d_G(u_i))^3 + \sum_{i=1}^{n_H-1}(d_H(v_i))^3 + \sum_{i=1}^{e_G}2^3 + (d_G(u) + d_H(v))^3 .$$

Then we have

$$\begin{aligned} F(\mathcal{S}_v) \quad &= \quad \sum_{i=1}^{n_G-1}(d_G(u_i))^3 + \sum_{i=1}^{n_H-1}(d_H(v_i))^3 + \sum_{i=1}^{e_G}2^3 + (d_G(u))^3 + (d_H(v))^3 \\ &\quad +3(d_G(u))^2 d_H(v) + 3d_G(u)(d_H(v))^2 \\ &= \quad F(G) - (d_G(u))^3 + F(H) - (d_H(v))^3 + 8e_G + (d_G(u))^3 \\ &\quad +(d_H(v))^3 + 3\big(d_G(u)d_H(v)\big)\big(d_G(u) + d_H(v)\big) \\ &= \quad F(G) + F(H) + 8e_G + 3\big(d_G(u)d_H(v)\big)\big(d_G(u) + d_H(v)\big). \end{aligned}$$

Note that for all vertices u in G, $\delta_G \leq d_G(u) \leq \Delta_G$ with equalities hold if and only if G is a regular graph. By replacing G by H, we obtain similar inequalities. Therefore, we have

$$F(\mathcal{S}_v) \leq F(G) + F(H) + 8e_G + 3\Delta_G\Delta_H\big(\Delta_G + \Delta_H\big)$$

and analogously $F(\mathcal{S}_v) \geq F(G) + F(H) + 8e_G + 3\delta_G\delta_H\big(\delta_G + \delta_H\big)$. Hence the result. □

Theorem 2.2. *A lower and an upper bound for the F-index of the R-vertex splice $\mathcal{S}_{vR}$ are given by*

$$F(\mathcal{S}_{vR}) \quad \leq 8F(G) + F(H) + 8e_G + 6\Delta_G\Delta_H\big(2\Delta_G + \Delta_H\big)$$

and

$$F(\mathcal{S}_{vR}) \quad \geq 8F(G) + F(H) + 8e_G + 6\delta_G\delta_H\big(2\delta_G + \delta_H\big).$$

Proof. By Eqn. (1), we have

$$\begin{aligned} F(\mathcal{S}_{vR}) &= \sum_{i=1}^{n_G-1}(2d_G(u_i))^3 + \sum_{i=1}^{n_H-1}(d_H(v_i))^3 + \sum_{i=1}^{e_G} 2^3 + (2d_G(u)+d_H(v))^3 \\ &= 8\sum_{i=1}^{n_G-1}(d_G(u_i))^3 + \sum_{i=1}^{n_H-1}(d_H(v_i))^3 + 8e_G + 8(d_G(u))^3 + (d_H(v))^3 \\ &\quad +6d_G(u)d_H(v)\Big(2d_G(u)+d_H(v)\Big) \\ &= 8F(G) - (2d_G(u))^3 + F(H) - (d_H(v))^3 + 8e_G + (2d_G(u))^3 + (d_H(v))^3 \\ &\quad +6\big(d_G(u)d_H(v)\big)\big(2d_G(u)+d_H(v)\big) \\ &= 8F(G) + F(H) + 8e_G + 6\big(d_G(u)d_H(v)\big)\big(2d_G(u)+d_H(v)\big). \end{aligned}$$

As in the proof of Theorem 2.1 in above, $\delta_G \leq d_G(u) \leq \Delta_G$ and $\delta_H \leq d_H(u) \leq \Delta_H$ such that equalities hold if and only if G (or H) is a regular graph. Then we get the bounds as indicated in the statement of theorem. □

2.2. **S-edge and R-edge splice.** As in the previous section, let us first define the S- and R-edge splice graphs to obtain the definite expressions of F-index of them. Thus, assume that G and H are two vertex disjoint graphs.

Definition 2.2. *Let $I(G) = \{p_1, p_2, p_3\}$ and $A(G) = \{q_1, q_2, q_3\}$. Let p_1 be the inserted vertex in an edge of the subdivision graph $S(G)$, let q_1 be the added vertex in $R(G)$ and let $x_1 \in V(H)$. Then the S-edge splice (correspondingly the R-edge splice) of G and H is denoted by $\mathcal{S}_e$ (correspondingly $\mathcal{S}_{eR}$) that is obtained from $S(G)$ (correspondingly $R(G)$) and one copy of H by identifying the vertices p_1 (correspondingly q_1) and x_1 of $S(G)$ (correspondingly $R(G)$) and H.*

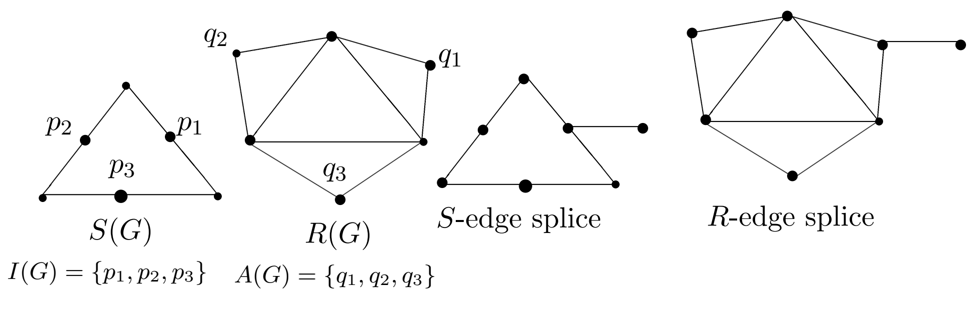

FIGURE 3. S-edge and R-edge splice graphs

Theorem 2.3. *The bounds for the F-index of S-edge splice are*

$$F(\mathcal{S}_e) \leq F(G) + F(H) + 8e_G + 6\Delta_H\big(\Delta_H + 2\big)$$

and

$$F(\mathcal{S}_e) \geq F(G) + F(H) + 8e_G + 6\delta_H\big(\delta_H + 2\big).$$

Proof. By Eqn. (1), we obtain

$$\begin{aligned} F(\mathcal{S}_e) &= \sum_{i=1}^{n_G}(d_G(u_i))^3 + \sum_{i=1}^{n_H-1}(d_H(v_i)^3 + \sum_{i=1}^{e_G-1} 2^3 + (d_H(v)+2)^3 \\ &= F(G)+F(H)-(d_H(v))^3+8(e_G-1)+(d_H(v))^3+8+6d_H(v)(d_H(v)+2) \\ &= F(G)+F(H)+8(e_G-1)+8+6d_H(v)(d_H(v)+2) \\ &= F(G)+F(H)+8e_G+6d_H(v)(d_H(v)+2) \end{aligned}$$

such that $\delta_G \leq d_G(u) \leq \Delta_G$. These imply the bounds in theorem, as required. □

On the other hand, again by Eqn. (1), we have the following result:

Theorem 2.4. *The bounds for the F-index of the R-edge splice $\mathcal{S}_{eR}$ are given by*

$$F(\mathcal{S}_{eR}) \quad \leq 8F(G)+F(H)+8e_G+6\Delta_H\big(2+\Delta_H\big)$$

and

$$F(\mathcal{S}_{eR}) \quad \geq 8F(G)+F(H)+8e_G+6\delta_H\big(2+\delta_H\big).$$

Proof.

$$\begin{aligned} F(\mathcal{S}_{eR}) &= \sum_{i=1}^{n_G}2(d_G(u_i))^3 + \sum_{i=1}^{e_G-1} 2^3 + \sum_{j=1}^{n_H-1}(d_H(v_j))^3 + (d_H(v)+2)^3 \\ &= 8F(G)+8(e_G-1)+F(H)-(d_H(v))^3+(d_H(v))^3+8 \\ &\quad +6d_H(v)\big(d_H(v)+2\big) \\ &= 8F(G)+F(H)+8e_G+6d_H(v)\big(2+d_H(v)\big) \end{aligned}$$

which implies that $F(\mathcal{S}_{eR}) \leq 8F(G)+F(H)+8e_G+6\Delta_H\big(2+\Delta_H\big)$. With a similar idea, we can also get the lower bound $F(\mathcal{S}_{eR}) \geq 8F(G)+F(H)+8e_G+6\delta_H\big(2+\delta_H\big)$. Hence the result. □

2.3. **S-vertex (-edge) neighborhood and R-vertex (-edge) neighborhood splices.** By using same construction and proof techniques as in the previous two sections, in this final part, we find the certain expressions for F-index of S-vertex neighborhood and R-vertex neighborhood splice graphs, and for F-index of S-edge neighborhood and R-edge neighborhood splice graphs, separately. Therefore we shall consider two vertex disjoint graphs G and H.

Definition 2.3. *Let $a_1 \in V(G)$ and $x_1 \in V(H)$. The S-vertex neighborhood $\mathcal{S}_{n_v}$ (correspondingly R-vertex neighborhood $\mathcal{S}_{n_vR}$) splice (NS) of G and H is obtained from $S(G)$ (correspondingly $R(G)$) and $d(a_1)$ copies of H by identifying the neighborhood vertices a_1 and x_1, (see Fig. 4).*

Let $p_1 \in I(G)$ be the inserted vertex of $S(G)$, let $q_1 \in A(G)$ be the added vertex of $R(G)$ and let $x_1 \in V(H)$. Then the S-edge neighborhood splice (correspondingly the R-edge neighborhood splice) of G and H is denoted by $\mathcal{S}_{n_e}$ (correspondingly $\mathcal{S}_{n_eR}$) and is obtained from $S(G)$ (correspondingly $R(G)$) and two copies of H by identifying the vertices p_1 (correspondingly q_1) and x_1, (see Fig. 5).

We have the following results:

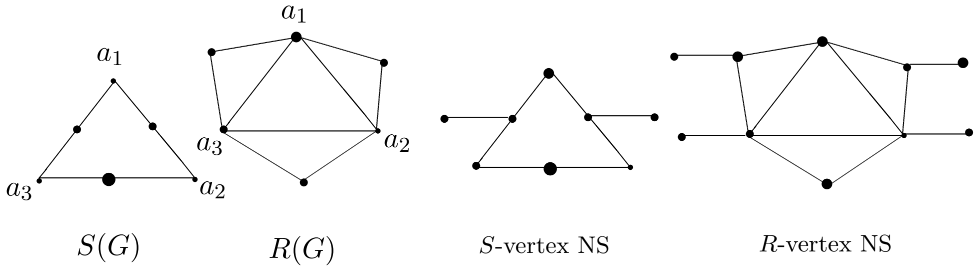

FIGURE 4. S- and R-vertex neighbourhood splices

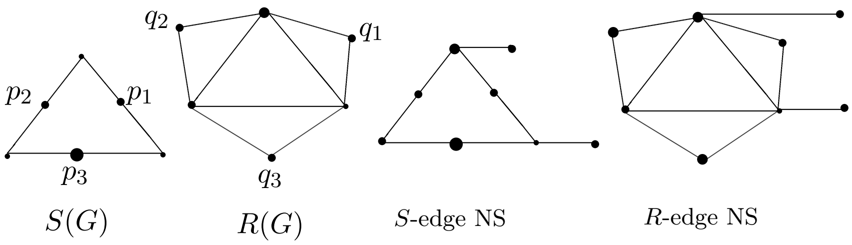

FIGURE 5. S- and R-edge neighbourhood splices

Theorem 2.5. *The bounds for the F-index of $\mathcal{S}_{n_v}$ and $\mathcal{S}_{n_e}$ are given by*

$$\left.\begin{aligned} F(\mathcal{S}_{n_v}) &\leq F(G) + \Delta_G F(H) + 8\Delta_G + 6\Delta_G\Delta_H\big(\Delta_H + 2\big) + 8e_G - 2 \\ F(\mathcal{S}_{n_v}) &\geq F(G) + \delta_G F(H) + 8\delta_G + 6\delta_G\delta_H\big(\delta_H + 2\big) + 8e_G - 2 \end{aligned}\right\} \tag{2}$$

and

$$\left.\begin{aligned} F(\mathcal{S}_{n_e}) &\leq F(G) + 2F(H) + 8e_G + 6\Delta_G\Delta_H\big(\Delta_G + \Delta_H\big) \\ F(\mathcal{S}_{n_e}) &\geq F(G) + 2F(H) + 8e_G + 6\delta_G\delta_H\big(\delta_G + \delta_H\big) \end{aligned}\right\}, \tag{3}$$

respectively.

Proof. The proof is based on Eqn. (1) as in above results.

$$\begin{aligned} F(\mathcal{S}_{n_v}) &= \sum_{i=1}^{n_G}(d_G(u_i))^3 + d_G(a_1)\sum_{j=1}^{n_H-1}(d_H(v_j))^3 + d_G(a_1)(d_H(v)+2)^3 + \sum_{i=1}^{e_G-2}(2)^3 \\ &= F(G) + d_G(a_1)F(H) - d_G(a_1)(d_H(v))^3 + d_G(a_1)(d_H(v))^3 \\ &+ 8d_G(a_1) + 6d_G(a_1)d_H(v)\bigg(d_H(v)+2\bigg) + 8(e_G-2) \\ &\leq F(G) + \Delta_G F(H) + 8\Delta_G + 6\Delta_G\Delta_H\big(\Delta_H+2\big) + 8e_G - 2 \end{aligned}$$

since $d_G(a_1) \leq \Delta_G$ and $d_H(v) \leq \Delta_H$ which gives the upper bound of (2). On the other hand,

$$\begin{aligned} F(\mathcal{S}_{n_e}) &= \sum_{i=1}^{n_G-2}(d_G(u_i))^3 + \sum_{i=1}^{e_G}(2)^3 + 2\sum_{j=1}^{n_H-1}(d_H(v_j))^3 + 2(d_G(u) + d_H(v)))^3 \\ &= F(G) - 2(d_G(u))^3 + 8e_G + 2F(H) - 2(d_H(v))^3 + 2(d_G(u))^3 \\ &+ 2(d_H(v))^3 + 3d_G(u)d_H(v)\big(d_G(u) + d_H(v)\big) \\ &= F(G) + 2F(H) + 8e_G + 6(d_G(u)d_H(v))\big(d_G(u) + d_H(v)\big) \\ &\leq F(G) + 2F(H) + 8e_G + 6\Delta_G\Delta_H\big(\Delta_G + \Delta_H\big) \end{aligned}$$

since $d_G(a_1) \leq \Delta_G$ and $d_H(v) \leq \Delta_H$ which gives the upper bound of (3).

Besides, the lower bounds indicated in (2) and (3) can be obtained easily again by Eqn. (1) and by the inequalities $d_G(a_1) \geq \delta_G$ and $d_H(v) \geq \Delta_H$. Hence the result. □

Additionally, we also have the following lower and upper bounds for $\mathcal{S}_{n_vR}$ and $\mathcal{S}_{n_eR}$:

Theorem 2.6. *The bounds for the F-index of $\mathcal{S}_{n_vR}$ and $\mathcal{S}_{n_eR}$ are given by*

$$\left.\begin{array}{ll} F(\mathcal{S}_{n_vR}) & \leq 8F(G) + 2\Delta_G F(H) + \Delta_G\Delta_H^3 + 6\Delta_G^2\Delta_H\big(2\Delta_G + \Delta_H\big) - 2\Delta_G\Delta_H^3 \\ & +\Delta_G\big(2+\Delta_H\big)^3 + 8\big(e_G - \Delta_G\big) \\ F(\mathcal{S}_{n_vR}) & \geq 8F(G) + 2\delta_G F(H) + \delta_G\delta_H^3 + 6\delta_G^2\delta_H\big(2\delta_G + \delta_H\big) - 2\delta_G\delta_H^3 \\ & +\delta_G\big(2+\delta_H\big)^3 + 8\big(e_G - \delta_G\big) \end{array}\right\} \tag{4}$$

and

$$\left.\begin{array}{ll} F(\mathcal{S}_{n_eR}) & \leq 8F(G) + 2F(H)) + 8e_G + 12\Delta_G\Delta_H\big(2\Delta_G + \Delta_H\big) \\ F(\mathcal{S}_{n_eR}) & \geq 8F(G) + 2F(H)) + 8e_G + 12\Delta_G\Delta_H\big(2\Delta_G + \Delta_H\big) \end{array}\right\}, \tag{5}$$

respectively.

Proof. Since $F(\mathcal{S}_{n_vR})$ can be written as

$$\sum_{i=1}^{n_G-d_G(a_1)} (2d_G(u_i))^3 + d_G(a_1)\big(2d_G(u) + d_H(v)\big)^3 + 2d_G(a_1)\sum_{j=1}^{n_H-1}(d_H(v_j))^3$$
$$+d_G(a_1)(2+d_H(v))^3 + \sum_{i=1}^{e_G-d_G(a_1)} (2)^3,$$

we clearly have

$$\begin{aligned} F(\mathcal{S}_{n_vR}) &= 8F(G) - 8d_G(a_1)(d_G(u))^3 + 8d_G(a_1)(d_G(u))^3 + d_G(a_1)(d_H(v))^3 \\ &\quad +6d_G(a_1)d_G(u)d_H(v)(2d_G(u)+d_H(v)) + 2d_G(a_1)F(G) - 2d_G(a_1)(d_H(v))^3 \\ &\quad +d_G(a_1)(2+d_H(v))^3 + 8(e_G - d_G(a_1)) \\ &= 8F(G) + d_G(a_1)(d_H(v))^3 + 6d_G(a_1)d_G(u)d_H(v)(2d_G(u)+d_H(v)) \\ &\quad +2d_G(a_1)F(G) - 2d_G(a_1)(d_H(v))^3 + d_G(a_1)(2+d_H(v))^3 + 8(e_G - d_G(a_1)). \end{aligned}$$

Thus, by taking into account $d_G(a_1) \leq \Delta_G$ and $d_H(v) \leq \Delta_H$, we obtain the first part of (4), and considering $d_G(a_1) \geq \delta_G$ and $d_H(v) \geq \delta_H$ we obtain the second part of (4).

By replacing the above calculations for $\mathcal{S}_{n_eR}$, and also considering same inequalities again, we get both the first and second part of Eqn. (5). Hence the result. □

Conclusion. In this paper, one of the graph operations which is related to RNA sequencing is studied and their forgotten index is calculated.

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Veerebradiah Lokesha for the photography and short autobiography, see TWMS J. App. Eng. Math., V.6, N.2, 2016

Sushmitha Jain received her M.Sc. degree with first rank and gold medallist from Vijayanagara Sri Krishnadevaraya University, Ballari in 2015. She has been pursuing her Ph. D. programme since 2016 in the Department of Studies in Mathematics, Vijayanagara Sri Krishnadevaraya University, Ballari. Her area of interest is chemical graph theory. She has published 6 research articles in International reputed Journals and presented research papers in 8 reputed conferences. She is the awardee of Maulana Azad National Fellowship for Minority Students.

Manjunath Muddalapuram graduated and received his M.Sc. degree from Gulbarga University, Gulbarga in 2012. He started his doctorate programme in 2016 from the Vijayanagara Sri Krishnadevaraya University. His area of interest is chemical graph theory. He has published 4 research articles in international reputed Journals and presented research articles in 10 reputed congresses. He is actively visiting IITs and reputed institutions for workshop and short visits for research work. He is the awardee of national fellowship and scholarship for higher studies of ST students (NO.: 201718-NFST-KAR-00838).

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Ismail Naci Cangul for the photography and short autobiography, see TWMS J. App. Eng. Math., V.6, N.2, 2016