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Forgotten Index and Forgotten Coindex of Graphs

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Abstract

F index is a connected graph, sum of the cubes of the vertex degrees. The forgotten topological index has been designed to be employed in the examination of drug molecular structures, which is extremely useful for pharmaceutical and medical experts in understanding the biological activities. Among all the topological indices, the forgotten index is based on degree connectivity on bonds. This paper characterized the forgotten index of union of graphs, join graphs, limits on trees and its complements, and accuracy is measured. Co-index values are analyzed for the various molecular structure of chemical compounds.

Keywords: Complement, Degree, Distance, Drugs, Graph, Molecular structure.

Introduction

Consider I, without several bonds and loops, is a graph. The graphs are the chemical structure model in which the atoms are treated as vertices and bonds are edges. Molecular topology is a numerical descriptor that characterizes the chemical graphs representing the chemical structure. Correla is the potential capacity of chemical compounds to produce a pharmacological and toxicological effect. Different types of bonds such as hydrogen depleted bonds, dipole bonds, and ionic bonds, hold together the atoms and molecules of all organic substances[1]. Among the bond connectivity indices, Furtula and Gutman examined the degree based index named forgotten index[2] or F-index $F(I) = \sum_{a\,\epsilon\, V(I)} \delta_I(a)^3 = \sum_{ab\,\epsilon\, E(I)} [\delta_I(a)^2 + \delta_I(b)^2]$, where $\delta_I(a)$denotes the degree of the vertex. Wei Gao et al analysed the chemical structures for forgotten index which are frequently used in drug molecular graphs[3]. In 2019, Mahdieh Azari and Farzaneh Falahati-nezhad calculated the exact formulae for forgotten topological coindex for some graphs[4]. Shehanaz and Muhammad Imran determined the formulas for forgotten index of four operations on graphs[5]. Akbar Jahanbani *et al* characterized the new results for forgotten coindex[6]. $\bar{F}\,(I) = \sum_{a\,\epsilon\, V(I)} \big(n-1-\delta_I(a)\big)\, \delta_I(a)^2$. In 2021, Mahmood Madian Abdullah *et al* were introduced thee schultz polynomial for chain and ring for square graphs[7]. Graph operations on corona product of graphs done by Adirasari RP et *al* [8]. This paper studies the forgotten index, forgotten coindex of union of graphs, join graph, bounds on tree and its complements and exact values of this index using Zagreb index $M_I(\mathrm{I}) = \sum_{\mathrm{a}\,\epsilon\, \mathrm{V(I)}} \delta_\mathrm{I}(\mathrm{a})^2 = \sum_{\mathrm{ab}\,\epsilon\, \mathrm{E(I)}} \big(\delta_\mathrm{I}(\mathrm{a}) + \delta_\mathrm{I}(\mathrm{b})\big)$[9]. Further analyze the forgotten coindex values and forgotten polynomial

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also calculated for different molecular structure of chemical compounds.

Materials and Methods

The forgotten coindex of $I_1 \cup I_2 \cup \ldots \cup I_k$ is denoted by $\cup_{i=1}^{k} I_i$ be a union of linked graph. The nodes of the graph $I_1 \cup I_2 \cup \ldots \cup I_k$ be $|V(I_1)| + |V(I_2)| + \ldots + |V(I_k)|$ and the links be $|E(I_1)| + |E(I_2)| + \ldots + |E(I_k)|$. Each associated k graph can be taken separately, then $\bar{F}(I_1 \cup I_2 \cup \ldots \cup I_k) = \bar{F}(I_1) + \bar{F}(I_2) + \ldots + \bar{F}(I_k)$.

Example 1: Let I_1 and I_2 be two connected graph as given in Fig 1.

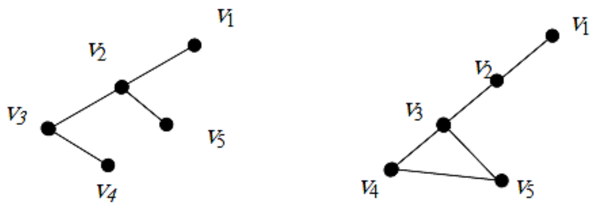

Figure 1. Disjoint union of the graphs I_1 and I_2

In the Fig 1, $\bar{F}(I_1) = 26, \bar{F}(I_2) = 36$ and $\bar{F}(I_1 \cup I_2) = 62$. For acyclic graph I, the complement of connected graph I depend on the degree sequence of graph I. If at least one vertex has degree one in the acyclic graph then the complement of I is disconnected. Graph I can be path P_4 or P_5 then $\bar{F}(I) = \bar{F}(\bar{I})$. The degree of the acyclic graph sequence is lower than its graph complement. Forgotten coindex which satisfies $\bar{F}(I) \leq \bar{F}(\bar{I})$.

Theorem 1: The acyclic graph I, $\bar{F}(\bar{I}) = 2(p-1)^3 + F(I) - 2(p-1)M_1(I)$.

Proof: Let I will be the degree sequence $g_1, g_2, \ldots, g_p$ of an acyclic graph. By the idea of forgotten coindex $\bar{F}(\bar{I}) = \sum_{ab \notin E(I)} \left(\delta_I^2(a) + \delta_I^2(b)\right)$, it is determined that the forgotten coindex any pair of vertices in I which are not connected between the vertices in coindex graph $\bar{I}$. The degree sequence of $\bar{I}$ being $\bar{g}_1, \bar{g}_2, \ldots, \bar{g}_p$.

$$\bar{F}(\bar{I}) = \sum_{ab \notin E(I)} \left[\left((\bar{g}_1(a))^2 + (\bar{g}_2(b))^2\right) + \left((\bar{g}_2(a))^2 + (\bar{g}_3(b))^2\right) + \ldots + \left(\left(\bar{g}_{p-1}(a)\right)^2 + \left(\bar{g}_{p-2}(b)\right)^2\right)\right]$$

$$\bar{F}(\bar{I}) = \left[((p-1-g_1)^2 + (p-1-g_2)^2) + \ldots + \left((p-1-g_{p-1})^2 + (p-1-g_p)^2\right)\right]$$

$$\bar{F}(\bar{I}) = \left[((p-1)^2 + g_1^2 - 2(p-1)g_1) + \ldots + ((p-1)^2 + g_p^2 - 2(p-1)g_p)\right]$$

$$\bar{F}(\bar{I}) = \underbrace{(p-1)^2 + (p-1)^2 + \ldots + (p-1)^2}_{2(p-1)} + \sum_{\substack{over\ all \\ edges\ ab \in E(I)}} \left[\left(\delta_I^2(a) + \delta_I^2(b)\right) + \ldots + \left(\delta_I^2(a) + \delta_I^2(b)\right)\right]$$

$$\bar{F}(\bar{I}) = \underbrace{(p-1)^2 + (p-1)^2 + \ldots + (p-1)^2}_{2(p-1)} + \sum_{\substack{over\ all \\ edges\ ab \in E(I)}} \left[\left(\delta_I^2(a) + \delta_I^2(b)\right) + \ldots + \left(\delta_I^2(a) + \delta_I^2(b)\right)\right]$$

$$-2(p-1)\left[\sum_{\substack{over\ all \\ edges\ ab \in E(I)}} \left[\left(\delta_I(a) + \delta_I(b)\right) + \ldots + \left(\delta_I(a) + \delta_I(b)\right)\right]\right]$$

$$\bar{F}(\bar{I}) = (p-1)^3 + \sum_{\substack{over\ all \\ edges\ ab \in E(I)}} \left(\delta_I^2(a) + \delta_I^2(b)\right) - 2(p-1) \sum_{\substack{over\ all \\ edges\ ab \in E(I)}} \left(\delta_I(a) + \delta_I(b)\right)$$

$$\bar{F}(\bar{I}) = 2(p-1)^3 + F(I) - 2(p-1)M_1(I).$$

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Theorem 2: The forgotten index and coindex of $P_r \odot P_s$ and $C_r \odot C_s$ be

$F(P_r \odot P_s) = r(8s+7) - 28$, $\bar{F}(P_r \odot P_s) = 4r^2s^2 - 22rs + 2r^2s - 14r + 48$ and

$F(C_r \odot C_s) = 4F(C_r) + 2r(20) + 8p(r-2)$,
$\bar{F}(C_r \odot C_s) = 12r^2s + 4r^2s^2 - 68r - 12rs$.

Proof: The graph $P_r \odot P_s$ is obtained from path P_r by merging a path P_s by all the vertices of path P_r. $|V(P_r \odot P_s)| = rs$, $|E(P_r \odot P_s)| = rs - 1$, Using degree sequence $rs - 2r + 2$ vertices has degree 2, s vertices has degree 1 and remaining s-2 vertices has degree 3.

$$F(P_r \odot P_s) = \Bigg[(2^2+3^2) + \underbrace{(3^2+3^2)+(3^2+3^2)+\ldots+(3^2+3^2)}_{(r-3)} + (2^2+3^2)$$

$$+ \underbrace{\underbrace{(2^2+2^2)+(2^2+2^2)+\ldots+(2^2+2^2)}_{(s-2)\ times}}_{r\ times} + (2^2+1^2)\Bigg]$$

$F(P_r \odot P_s) = 18(r-3) + 26 + 8r(s-2) + 5r = r(8s+7) - 28.$

The forgotten coindex of $P_r \odot P_s$ be

$$\bar{F}(\mathrm{P_r} \odot \mathrm{P_s}) = \Bigg[(rs-3)2^2 + \underbrace{(rs-4)3^2 + (rs-4)3^2 + \ldots + (rs-4)3^2}_{(r-2)\ times} + (rs-3)2^2$$

$$+ \underbrace{\underbrace{(rs-3)2^2 + \ldots + (rs-3)2^2}_{\mathrm{r\ times}}}_{\mathrm{(rs-2r)\ times}} + \underbrace{(\mathrm{rs}-2)+\ldots+(\mathrm{rs}-2)}_{\mathrm{r\ times}}\Bigg]$$

$\bar{\mathrm{F}}(\mathrm{P_r} \odot \mathrm{P_s}) = (\mathrm{rs} - 2\mathrm{r} + 2)(\mathrm{rs} - 3)2^2 + (\mathrm{r} - 2)(\mathrm{rs} - 4)3^2 + \mathrm{r}(\mathrm{rs} - 2)$

$\bar{\mathrm{F}}(\mathrm{P_r} \odot \mathrm{P_s}) = 4\mathrm{r}^2\mathrm{s}^2 - 22\mathrm{rs} + 2\mathrm{r}^2\mathrm{s} - 14\mathrm{r} + 48$

The graph $C_r \odot C_s$ is obtained from cycle C_r by gluing a cycle C_s by all the vertices of cycle C_r, $|V(C_r \odot C_s)| = r(s-1)$, $|E(C_r \odot C_s)| = r(s+1)$.

Using degree sequence r vertices has degree 4 and $r(s-1)$ vertices has degree 2.

$$F(C_r \odot C_s) = [(4^2+4^2)+(4^2+4^2)+\ldots+(4^2+4^2)$$

$$+ \underbrace{(4^2+2^2) + \underbrace{(2^2+2^2)+(2^2+2^2)+\ldots+(2^2+2^2)}_{(s-2)\ times} + (4^2+2^2)}_{r\ times}\Bigg]$$

$F(C_r \odot C_s) = 4F(C_r) + 2r(20) + p(r-2)8$

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The forgotten coindex of $C_r \odot C_s$ be

$$\bar{F}(C_r \odot C_s) = \left[\underbrace{(rs-5)4^2 + (rs-5)4^2 + \ldots + (rs-5)4^2 + (rs-3)2^2 + (rs-3)2^2 + \ldots + (rs-3)2^2}_{r\ times}\right]$$

$$\bar{F}(C_r \odot C_s) = \left[\underbrace{(rs-5)4^2 + (rs-5)4^2 + \ldots + (rs-5)4^2}_{r\ times} + \underbrace{(rs-3)2^2 + (rs-3)2^2 + \ldots + (rs-3)2^2}_{r(s-1)\ times}\right]$$

$$\bar{F}(C_r \odot C_s) = [r(rs-5)4^2 + r(s-1)(rs-3)2^2]$$

$$\bar{F}(C_r \odot C_s) = 12r^2s + 4r^2s^2 - 68r - 12rs.$$

Theorem 3: $F[G(p,q) \odot P_m] = F(G) + 3M_1(G) - 14p + 6q + 8pm.$

Proof: Let $G(p,q)$ be a graph with degree sequence $g_1, g_2, \ldots, g_p$. The graph $G(p,q) \odot P_m$ is obtained from $G(p,q)$ by merging a path P_m by all the vertices of $G(p,q)$. $|V(G(p,q) \odot P_m)| = pm$ and $|E(G(p,q) \odot P_m)| = pm - p + q$.

$$F[G(p,q) \odot P_m] = \sum_{ab \in F[G(p,q) \odot P_m]} [(g_1(a)^2 + g_2(b)^2) + (g_2(a)^2 + g_3(b)^2) + \ldots . + (g_{p-1}(a)^2 + g_p(b)^2)$$

$$+ \left[(g_1{}^2 + 2^2) + \underbrace{(2^2 + 2^2) + \ldots + (2^2 + 2^2)}_{(m-3)\ times} + (2^2 + 1^2)\right] + \ldots$$

$$+ \left[(g_p{}^2 + 2^2) + \underbrace{(2^2 + 2^2) + \ldots + (2^2 + 2^2)}_{(m-3)\ times} + (2^2 + 1^2)\right]$$

$$F[G(p,q) \odot P_m] = \left[(g_1 + 1)^2 + (g_2 + 1)^2 + \ldots + (g_p + 1)^2\right]$$

$$+ \left[(g_1{}^2 + 2^2) + (g_2{}^2 + 2^2) + \ldots + (g_p{}^2 + 2^2)\right]$$

$$+ \left[\underbrace{(2^2 + 2^2) + (2^2 + 2^2) + \ldots + (2^2 + 2^2)}_{p(m-3)\ times}\right]$$

$$+ \left[\underbrace{(2^2 + 1^2) + (2^2 + 1^2) + \ldots + (2^2 + 1^2)}_{p\ times}\right]$$

$$F[G(p,q) \odot P_m] = F(G) + 2M_1(G) + 2q + M_1(G) + 4q + 5p + 8p(m-3) + 5p$$

$$F[G(p,q) \odot P_m] = F(G) + 3M_1(G) - 14p + 6q + 8pm.$$

Theorem 4: The Mycielski construction of path and cycle graph $[\chi(P_p)] = p^3 + 91p - 150$, $F[\chi(C_p)] = p^3 + 91p$.

Proof: The Mycielski construction of path graph has $2p + 1$ vertices and $4p - 3$ edges. Among that $p - 2$ vertices has degree 4, 4 vertices has degree 2 and one vertex has degree p. Using the degree sequence Mycielski construction of path graph is

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$$F[\chi(P_p)] = \left[(2^2+4^2) + \underbrace{(4^2+4^2)+(4^2+4^2)+\ldots+(4^2+4^2)}_{(n-3)\ times} + (2^2+4^2)\right]$$

$$+\left[(2^2+4^2)+(2^2+3^2)+\underbrace{(3^2+4^2)+(3^2+4^2)+\ldots+(3^2+4^2)}_{2(p-1)\ times}+(2^2+4^2)+(2^2+3^2)\right]$$

$$+\left[(2^2+p^2) + \underbrace{(3^2+p^2)+(3^2+p^2)+\ldots+(3^2+p^2)}_{(p-2)\ times}+(2^2+p^2)\right]$$

$$F[\chi(P_p)] = [32(p-3)+40+25(2p-6)+40+26 + p^3+8+9(p-2)]$$

$$F[\chi(P_p)] = p^3+91p-150.$$

Mycielski construction of cycle graph $\chi(C_p)$, p vertices has degree 4, p vertices has degree 3 and a vertex has degree p.

$$F[\chi(C_p)] = \left[\underbrace{(4^2+4^2)+\ldots+(4^2+4^2)}_{p\ times} + \underbrace{(4^2+3^2)+\ldots+(4^2+3^2)}_{2p\ times} + \underbrace{(3^2+6^2)+\ldots+(3^2+6^2)}_{p\ times}\right]$$

$$F[\chi(C_p)] = p(4^2+4^2)+2p(4^2+3^2) + p(3^2+6^2)$$

$$F[\chi(C_p)] = p^3+91p.$$

Example 2: In Fig 2, the forgotten index for mycielski construction of cycle graph C_6 is 762.

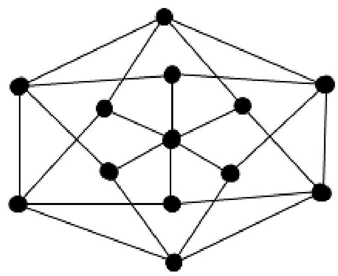

Figure 2. Mycielski construction of cycle graph $\chi(C_6)$

Results and Discussion

Antiviral Compounds:

Ribavirin has a specific dimensional governing DNA and RNA viruses. It is an antibacterial agent for the prevention of infection through RSV. The molecular structure of ribavirin is shown in Fig 3. In Fig 4, Valganciclovir is the small molecular substance that can be treated against infections including cytomegaloviruses. Currently, it is prodrug towards ganciclovir. It is rapidly converted by digestive as well as gastric enzymes to acyclovir after orally administrated. Thymidine is a pyrimidine 2'- deoxyribonucleoside that has thymine as the nucleobase in Fig 5. The drugs aspartame, oxprenolol and chrysinare in Figs 6, 7 and 8. It has a function as a metabolite, a human metabolite, an Escherichia coli metabolite of a mouse.

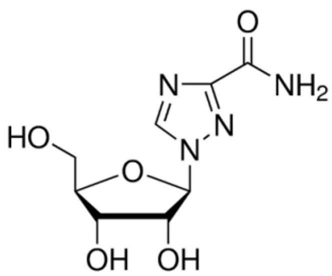

Figure 3. The molecular structure Ribavirin

Table 1, follows the antiviral compounds of the forgotten index and coindex can be calculated. The antiviral compounds are directly proportional to the forgotten index and forgotten coindex. If the

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antiviral compounds are acyclic graphs, then the forgotten index is greater than the coindex.

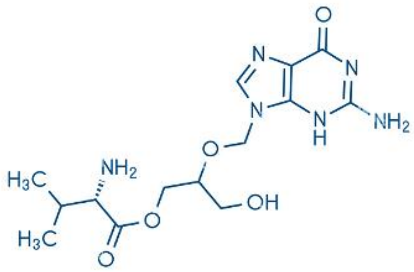

Figure 4. The molecular structure Valganciclovir

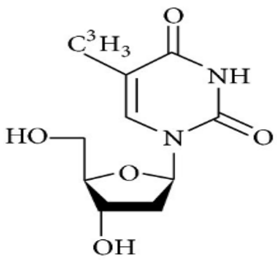

Figure 5. The molecular structure b-Thymidine

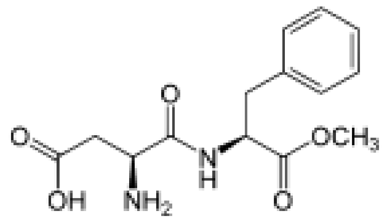

Figure 6. The molecular structure Aspartame

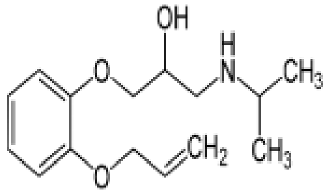

Figure 7. The molecular structure Oxprenolol

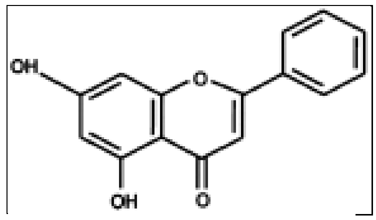

Figure 8. The molecular structure Chrysin

Table 1. Antiviral compounds of forgotten index and forgotten coindex.

Antiviral drugs	Forgotten Index F(I)	Forgotten Coindex $\overline{F}(I)$
Ribavirin	166	597
Valganciclovir	297	2318
b-Thymidine	204	770
Aspartame	208	1490
Oxprenolol	180	1146
Chrysin	211	1126

Conclusion

The measures of forgotten index and coindex were characterized and solved the operation of gluing graphs and also characterized the Mycielski conjecture of path and cycle graphs and also analyzed the antiviral drugs of Ribavirin, Valganciclovir, b-Thymidine, Aspartame, Oxprenolol, and Chrysin. The vivo work may be required to certificate the effectiveness and safety of these inhibitors against SARS-CoV-2.

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Author's Declaration

- Conflicts of Interest: None.
- We hereby confirm that the Figures and Table in the manuscript are ours. Besides, the Figures and

Images, which are not ours, have been given the permission for re-publication attached with the manuscript.

- Ethical Clearance: The project was approved by the local ethical committee in Vel Tech Rangarajan Dr Sagunthala R & D Institute of Science and Technology, India.

Author's Contribution Statement

This work was carried out in collaboration between all authors. J S and A M analysed the antiviral compounds and numerical values were calculated. All authors read and approved the final manuscript.

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الفهرس المنسي و المؤشر الثانوي المنسي للرسوم البيانية

ج . سنباجا مالار ، أ- ميناكشي

قسم الرياضيات ، معهد تك فال رانجاراجان د. ساكنثال ر. اند د. للعلوم والتكنولوجيا ، تاميل نادو ، الهند.

الخلاصة

مؤشر F هو رسم بياني متصل ، مجموع مكعبات درجات الرأس. تم تصميم الفهرس الطوبولوجي المنسي ليتم استخدامه في فحص الهياكل الجزيئية للعقار، وهو مفيد للغاية لخبراء الأدوية والطب في فهم الأنشطة البيولوجية. من بين جميع المؤشرات الطوبولوجية ، يعتمد المؤشر المنسي على درجة اتصال السندات. وصفت هذه الورقة الفهرس المنسي لاتحاد الرسوم البيانية ، والرسوم البيانية المرتبطة، وحدود الأشجار ومكملاتها ، ويتم قياس الدقة. يتم تحليل قيم الفهرس المشترك للتركيب الجزيئي المختلف للمركبات الكيميائية.

الكلمات المفتاحية: المكمل ، الدرجة ، المسافة ، الأدوية ، الرسم البياني ، التركيب الجزيئي.