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Interpolation method for computing some topological indices

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Abstract

Interpolation polynomials are suitable tools for calculating the topological indices of infinite series of molecular graphs. In this article, using interpolation polynomials, the Zagreb and Forgotten indices of a number of graph families are calculated.

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1. Introduction

A simple graph $G=(V,E)$ is a molecular graph, if its vertices correspond to atoms and edges correspond to bonds. The degree of a molecular graph G, ($d_G(v)$), is the number of bonds incident with v.

One of the most important topics in chemistry is the relationship between the properties of molecules and their characteristics. In this regard, graph theory has been able to play an important role [4, 5].

Chemical graph theory is the mathematical modeling of chemical structures with graph theory, which deals with the analysis of consequences related to chemical systems.

Quantitative structure-activity relationship (QSAR) is a method for building mathematical models to predict reactivity and investigate the properties of molecules and the numerical relationship between the activity of chemical compounds and their structure. This method is used in topological indices, genetics, artificial neural networks, drug design, toxicology and other physicochemical parameters [12, 14, 15].

Topological indices are real numbers that are attributed to molecular graphs, and are used to study the chemical and physical properties of molecules. To see some degree and distance based topological indices in a graph in biological sciences, physical - chemistry and QSAR studies we refer the readers to [1, 2, 3, 4, 5, 6, 11].

One of the main concepts in topological indices is the Zagreb index, which was introduced in 1972 by Gutman and $Trinajstić$ [10, 15] and defined as follows:

$$M_1(G)=\sum_{v\in V(G)} d_G^2(v)=\sum_{uv\in E(G)}[d_G(u)+d_G(v)]\ ,$$

and

$$M_2(G)=\sum_{uv\in E(G)} d_G(u)\, d_G(v)\ .$$

Due to the importance and applications of this index, researchers in their QSPR and QSAR studies conducted many researches about this index, some of which can be seen in [6, 13, 15, 16].

In the article [10], Gutman and his colleague defined another topological index, but the detailed study of this index was later carried out in the article [9] by Furtula and Gutman, and they called it F-index and defined as follows:

$$F(G)=\sum_{v\in V(G)} d_G^3(v)=\sum_{uv\in E(G)}[d_G^2(u)+d_G^2(v)]\ .$$

In this paper, we intend to use the concept of interpolation to find closed formulas for calculating some topological indices for some families of molecular graphs. For more information on this, we refer reader to papers [7] and [8].

2. Compute topological indices with interpolation of the functions with one variable

Suppose $a_1, a_2, a_3, \ldots$ are a sequence of real numbers in the form $A = \{a_n\}_{n\geq 1}$. We define, $D(A) = \{a_{n+1} - a_n\}_{n\geq 1}$ which, D(A) is named the first-order differences of A. The first-order differences of D(A) are named the second-order differences of A and denoted by $D^2(A)$. The $rth-order$ differences of A denoting by $D^r(A)$, is the first-order differences of $D^{r-1}(A)$. We finish definition and notations by contracting $D^0(A) = A$.

To calculate some topological indices, for a sequence of integers denoted by $A = \{a_n\}$, $n \geq 1$, if the sequences of $D^{K-1}(A)$ are non-constant while $D^K(A)$ is constant, then A is generated by a polynomial of degree k (see [8]).

Since our goal is to find a closed formula in polynomial form in a family of molecular graphs, as stated at the beginning of this section, it is sufficient to calculate the sequence of differences until a constant sequence is reached. If no such sequence is found, we claim that the closed formula cannot be calculated in polynomial form.

In the rest of this section, we will calculate the first and second Zagreb indices, and the F-index for windmill graph $D_3^{(m)}$, circumcoronene series of benzenoid H_k for $k \geq 1$, Fence graph $P_n[P_2]$, Closed Fence graph $C_n[P_2]$, Line graph of the subdivision graph of a Ladder graph L_n, and Triangular graph G_n , $n = 1, 2, 3, \ldots$.

Theorem 2.1: *The first and second Zagreb indices and F-index of windmill graph $D_3^{(m)}$ (see Figure 1) is computed as:*

a) $\mathrm{M}_1\left(\mathrm{D}_3^{(\mathrm{m})}\right) = 4\mathrm{m}^2 + 8\mathrm{m}$

b) $M_2\left(D_3^{(m)}\right) = 8m^2 + 4m$

c) $\mathrm{F}\left(\mathrm{D}_3^{(\mathrm{m})}\right) = 8\mathrm{m}^3 + 16\mathrm{m}$.

Proof: **(a).** A simple calculation shows the sequence of the first six values of $M_1\left(D_3^{(m)}\right)$, $m = 1, 2, \ldots, 6$ and the sequences of differences of consecutive terms are as follow,

$$\begin{gathered} A = \{12, 32, 60, 96, 140, 192, \ldots\} \\ D(A) = \{20, 28, 36, 44, 52, \ldots\} \\ D^2(A) = \{8, 8, 8, 8, \ldots\}. \end{gathered} \tag{1}$$

We show the sequence A is generated via a polynomial of degree two such as $P(m) = a_1 m^2 + a_2 m + a_3$. Sequences consist of variables of $P(m)$ where $m = 1, 2, 3, 4, 5, \ldots$ and their differences are,

$$\begin{aligned} A' = \{&a_1 + a_2 + a_3, 4a_1 + 2a_2 + a_3, 9a_1 + 3a_2 + a_3, 16a_1 + 4a_2 + a_3, 25a_1 \\ &+ 5a_2 + a_3, \ldots\} \end{aligned}$$

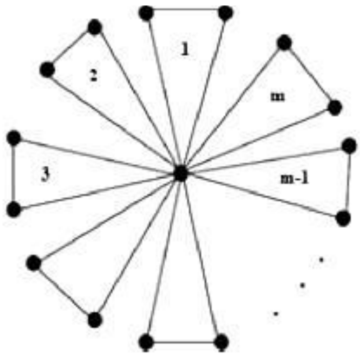

Figure 1
Windmill graph $D_3^{(m)}$

$$D(A') = \{3a_1 + 2a_2, 5a_1 + a_2, 7a_1 + a_2, 9a_1 + a_2, \dots\}, \quad (2)$$
$$D^2(A') = \{2a_1, 2a_1, 2a_1, \dots\}.$$

Comparing the corresponding sequences in (1) and (2) we have the following system of equations:

$$\begin{cases} a_1 + a_2 + a_3 = 12 \\ 3a_1 + a_2 = 20 \\ 2a_1 = 8 \end{cases}$$

and its solution is $a_1 = 4,\ \ a_2 = 8,\ a_3 = 0$ **.** From this, we get

$$\mathrm{M}_1\big(\mathrm{D}_3^{(\mathrm{m})}\big) = 4\mathrm{m}^2 + 8\mathrm{m}.$$

(b). The first 4 values of $M_2(\mathrm{D}_3^{(\mathrm{m})})$ is given as 12, 40, 84, 144, ….

Using the sequence $A = \{12, 40, 84, 144, \dots\}$ we get $D(A) = \{28, 44, 60, \dots\}$ and $D^2(A) = \{16, 16, \dots\}$. Now, we compare the above sequences with the sequences of the first three values of general polynomial given in (a); Hence

$$\begin{cases} a_1 + a_2 + a_3 = 12 \\ 3a_1 + a_2 = 28 \\ 2a_1 = 16 \end{cases}$$

So, we get

$$a_1 = 8, \qquad a_2 = 4, \qquad a_3 = 0\ .$$

Therefore, we have

$$M_2\big(D_3^{(m)}\big) = 8m^2 + 4m.$$

(c). We compute the sequence of the first six values of $F(D_3^{(m)})$ and the sequences of differences of consecutive terms are as follow,

$$A = \{24, 96, 264, 576, 1080, 1824, \dots\}$$

$$D(A) = \{72, 168, 312, 504, 744, \dots\}$$
$$D^2(A) = \{96, 144, 192, 240, \dots\}$$
$$D^3(A) = \{48, 48, 48, \dots\}.$$

Since the sequential differences after three steps end with the constant sequence, we conclude that $F(D_3^{(m)})$ has a cubic polynomial. It's easy to see that, the sequence A is generated via a polynomial of degree three such as $P(m) = a_1m^3 + a_2m^2 + a_3m + a_4 \ \ where\ m = 1, 2, 3, 4, 5, 6, \dots$. Sequences consist of variables of $P(m)$ and their differences are,

$$A' = \{a_1 + a_2 + a_3 + a_4, 8a_1 + 4a_2 + 2a_3 + a_4, 27a_1 + 9a_2 + 3a_3 + a_4, 64a_1 + 16a_2 + 4a_3 + a_4, 125a_1 + 25a_2 + 5a_3 + a_4, 216a_1 + 36a_2 + 6ca_3 + a_4, \dots\}$$

$$D(A') = \{7a_1 + 3a_2 + a_3, 19a_1 + 5a_2 + a_3, 37a_1 + 7a_2 + a_3, 61a_1 + 9a_2 + a_3, 91a_1 + 11a_2 + a_3, \dots\}$$
$$D^2(A') = \{12a_1 + 2a_2, 18a_1 + 2a_2, 24a_1 + 2a_2, 30a_1 + 2a_2, \dots\}$$
$$D^3(A') = \{6a_1, 6a_1, 6a_1, 6a_1, \dots\}.$$

By comparing the general sequence of polynomial with degree three, we get:

$$\begin{cases} a_1 + a_2 + a_3 + a_4 = 24 \\ 7a_1 + 3a_2 + a_3 = 72 \\ 12a_1 + 2a_2 = 96 \\ 6a_1 = 48\,. \end{cases}$$

Hence, $a_1 = 8, \quad a_2 = 0, \quad a_3 = 16, \quad a_4 = 0$. Therefore, we have

$$\mathrm{F}\left(\mathrm{D}_3^{(\mathrm{m})}\right) = 8\mathrm{m}^3 + 16\mathrm{m}.$$

Theorem 2.2: *The first and second Zagreb indices and F-index of* $circumcoronene$ *series of benzenoid* H_K *for* $k \geq 1$ *(see Figure 2) is computed as:*

(a) $\mathrm{M}_1(H_K) = 54\mathrm{k}^2 - 30\mathrm{k}$

(b) $M_2(H_K) = 81k^2 - 63k + 6$

(c) $\mathrm{F}(H_K) = 162\mathrm{k}^2 - 114\mathrm{k}$

Proof: **(a).** We compute the sequence of the first five values of $\mathrm{M}_1(H_K)$ and the sequences of differences of consecutive terms are as follow,

$$A = \{24, 156, 396, 744, 1200, \dots\}$$
$$D(A) = \{132, 240, 348, 456, \dots\}$$
$$D^2(A) = \{108, 108, 108, \dots\}.$$

Now, we compare the above sequences with the sequences of the first three values of general polynomial given in proof (a) of Theorem 2.1. Hence

$$\begin{cases} a_1 + a_2 + a_3 = 24 \\ 3a_1 + a_2 = 132 \\ 2a_1 = 108 \end{cases}$$

and, the solution is $a_1 = 54,\ \ a_2 = -30,\ \ \ a_3 = 0.$

Therefore, we have,

$$M_1(\mathrm{H}_k) = 54\mathrm{k}^2 - 30\mathrm{k}.$$

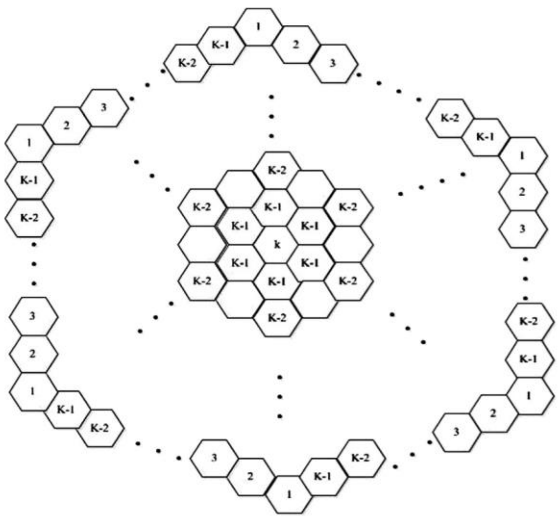

Figure 2
The circumcoronene series of benzenoid H_k for $k \geq 1$

(b). We compute the sequence of the first five values of $\mathrm{M}_2(H_K)$ and the sequences of differences of consecutive terms are as follow:

$$A = \{24, 204, 546, 1050, 1716, \dots\}$$
$$D(A) = \{180, 342, 504, 666, \dots\}$$
$$D^2(A) = \{162, 162, 162, \dots\}$$

And, the following system of equations is obtained:

$$\begin{cases} a_1 + a_2 + a_3 = 24 \\ 3a_1 + a_2 = 180 \\ 2a_1 = 162\ \ . \end{cases}$$

Hence $a_1 = 81,\ \ a_2 = -63,\ \ \ a_3 = 6$ **.** Therefore, we have

$$M_2(\mathrm{H}_k) = 81\mathrm{k}^2 - 63\mathrm{k} + 6.$$

(c). The sequence of index values for first five values of $F(H_k)$ is

$$\mathrm{A} = \{48, 420, 1116, 2136, 3480, \dots\}$$

and difference sequences of A are, $D(A) = \{372, 696, 1020, 1344, \ldots\}$ and $D^2(A) = \{324, 324, 324, \ldots\}$. Analogously with general polynomial given in proof (a) of theorem 2.1 we have:

$$\begin{cases} a_1 + a_2 + a_3 = 48 \\ 3a_1 + a_2 = 372 \\ 2a_1 = 324 \end{cases}.$$

Hence $a_1 = 162$, $a_2 = -114$, $a_3 = 0$. From this we get

$$F(H_k) = 162k^2 - 114k.$$

Since the proof of the following theorems is similar to the above theorems, we omit their proof.

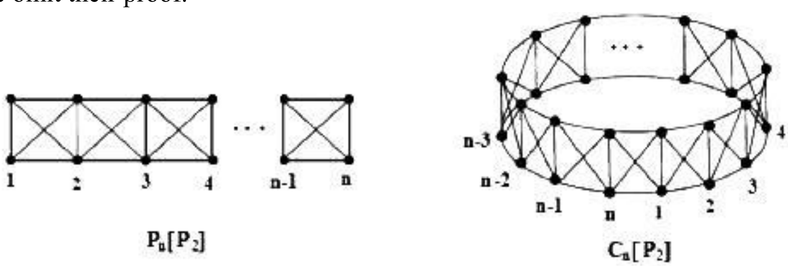

Figure 3
Fence and Closed fence graph

Theorem 2.3: *For the Fence graph $P_n[P_2]$ where $n \geq 2$ and integer (See Figure 3), prove*

$$M_1(P_n[P_2]) = 50n - 64$$

$$M_2(P_n[P_2]) = \begin{cases} 54 & \text{if} \quad n = 2 \\ 125n - 212 & \text{if} \quad n > 2 \end{cases}$$

$$F(P_n[P_2]) = 250n - 392.$$

Theorem 2.4: *For the Closed Fence graph $C_n[P_2]$ where $n \geq 3$ and integer (See Figure 3), then*

$$M_1(C_n[P_2]) = 50n$$

$$M_2(C_n[P_2]) = 125n$$

$$F(C_n[P_2]) = 250n.$$

The graph resulting from the Cartesian product of $P_n \times P_2$ in which $n \geq 1$ and integer, is called ladder graph and is denoted by L_n (See Figure 4).

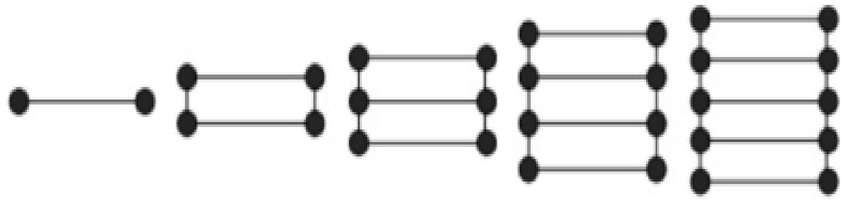

Figure 4
Ladder graphs $L_1,\ L_2,\ L_3,\ L_4,\ L_5$

Theorem 2.5: *Suppose G is the line graph of the subdivision graph of a Ladder graph L_n where $n \geq 1$ and integer, then:*

$$M_1(G) = \begin{cases} 2 & \text{if} \quad n = 1 \\ 54n - 76 & \text{if} \quad n \geq 2 \end{cases}$$
$$M_2(G) = \begin{cases} 1 & \text{if} \quad n = 1 \\ 32 & \text{if} \quad n = 2 \\ 81n - 132 & \text{if} \quad n \geq 3 \end{cases}$$
$$F(G) = \begin{cases} 2 & \text{if} \quad n = 1 \\ 162n - 260 & \text{if} \quad n \geq 2 \end{cases}.$$

Figure 5 shows a number of simple triangular graphs. The number of vertices of each of these simple triangular graphs G_n is given by the formula $\frac{(n+1)(n+2)}{2}$ and G_n consists of n^2 triangles enclosed in a larger triangle.

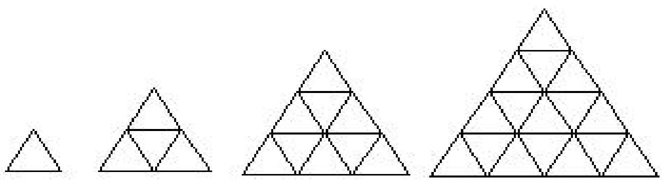

Figure 5
Triangular graphs G_n, $(n = 1, 2, 3, 4)$

Theorem 2.6: *For a simple triangle graph G_n, $n \geq 0$ and integer, the first and second Zagreb indices and F-index is computed as:*

$$M_1(G_{n+1}) = 18n^2 + 30n + 12$$
$$M_2(G_{n+1}) = 54n^2 + 30n + 12$$
$$F(G_{n+1}) = 108n^2 + 84n + 24.$$

3. Compute F-index with interpolation of the functions with two variables

In this section, according to the information in Table 1, we obtain closed formula for forgotten topological index of the 2D-Lattice, nanotube and nano-torus of TUC_4C_8[p, q] and Tadpole graph with interpolation of a function with two variable values.

Table 1
Number of vertices and edges

Graph	Number of vertices	Number of edges
2D-Lattice of TUC_4C_8[p, q]	4pq	6pq-p-q
TUC_4C_8[p, q] nanotube	4pq	6pq-p
TUC_4C_8[p, q] nano-torus	4pq	6pq

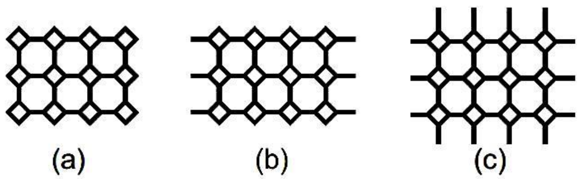

Figure 6
(a) 2D-Lattice of TUC_4C_8[4, 3], (b) TUC_4C_8[4, 3] nanotube, (c) TUC_4C_8[4, 3] nano-torus

Theorem 3.1:

(a) *If G be a graph of the 2D-Lattice of $TUC_4C_8[p,q]$ (See Figure 6 – (a)), then, the forgotten topological index of G is equal to*

$$F(G) = 108pq - 38p - 38q.$$

(b) *If G be a graph of the $TUC_4C_8[p,q]\ nanotube$ (see Figure 6-(b)), then, the F-index of G is equal to*

$$F(G) = 108pq - 38p.$$

(c) *If G be a graph of the $TUC_4C_8[p,q]\ nano-torus$ (see Figure 6-(c)), then, the F-index of G is equal to*

$$F(G) = 108pq.$$

Proof: Since proof of parts (a), (b), (c) are similar, then we proof part (a), and omit the proof of parts (b) and (c).

(a) The sequence of F-index values for $[p,q] = [0,0], [0,1], [1,0], [1,1]$ is as follows:

$$F(TUC_4C_8[0,0]) = 0, \qquad F(TUC_4C_8[0,1]) = -38,$$
$$F(TUC_4C_8[1,0]) = -38, \qquad F(TUC_4C_8[1,1]) = 32.$$

According to results obtained of [7], there is a unique interpolation polynomial of the degree n in the variable value x also y and has the form:

$$\begin{aligned} P_n(x,y) = a_{0,0} &+ a_{1,0}(x-x_0) + a_{0,1}(y-y_0) + a_{2,0}(x-x_0)(x-x_1) \\ &+ a_{1,1}(x-x_0)(y-y_0) + a_{0,2}(y-y_0)(y-y_1) + \cdots \\ &+ a_{n,0}(x-x_0)(x-x_1)\dots(x-x_{n-1}) \\ &+ a_{n-1,1}(x-x_0)(x-x_1)\dots(x-x_{n-2})(y-y_0) \\ &+ a_{n-2,2}(x-x_0)\dots(x-x_{n-3})(y-y_0)(y-y_1) + \cdots \\ &+ a_{0,n}(y-y_0)(y-y_1)\dots(y-y_{n-1}). \end{aligned} \tag{1}$$

The coefficients of this polynomial are determined by means of the next conditions:

$$\begin{cases} \mathrm{P_n}(x_i,y_0) = f(x_i,y_0) \;\; pentru \;\; i \in \{0,1,\dots,n\} \\ P_n(x_i,y_1) = f(x_i,y_1) \; pentru \;\; i \in \{0,1,\dots,n-1\} \\ \vdots \\ P_n(x_i,y_{n-1}) = f(x_i,y_{n-1}) \; pentru \;\; i \in \{0,1\} \\ P_n(x_0,y_n) = f(x_0,y_n \end{cases} \tag{2}$$

and, the divided differences are:

$$f[x_1] = f(x_1) \;\; , \;\; f[x_1,x_2] = \frac{f(x_2)-f(x_1)}{x_2-x_1} \;\; , \dots , \text{and}$$

$$f[x_1,x_2,\dots,x_k] = \frac{f[x_2,\dots,x_k]-f[x_1,\dots,x_{k-1}]}{x_k-x_1}.$$

Then for $i,j \in \{0,1,\dots,n\}$ and $i+j \le n$ we have

$$\begin{cases} f[x_i;y_j] = f(x_i,y_j); \\ f[x_0,x_1;y_j] = \frac{f[x_1,y_j]-f[x_0,y_j]}{x_1-x_0}; \\ f[x_i;y_j,y_{j+1}] = \frac{f[x_i,y_{j+1}]-f[x_i,y_j]}{y_{j+1}-y_j}; \\ \vdots \\ f[x_0,x_1,\dots,x_i;y_0,y_1,\dots,y_j] = \frac{f[x_0,x_1,\dots,x_i;y_1,\dots,y_j]-f[x_0,x_1,\dots,x_i;y_0,y_1,\dots,y_{j-1}]}{y_j-y_0} \\ \qquad = \frac{f[x_1,x_2,\dots,x_i;y_0,y_1,\dots,y_j]-f[x_0,x_1,\dots,x_{i-1};y_0,y_1,\dots,y_j]}{x_i-x_0}. \end{cases}$$

Considering the conditions (2) on the polynomial (1), we find:

$$\begin{aligned} &a_{i,0} = f[x_0,\, x_1,\dots,x_i;y_0] \;\; pentru \;\;\; i \in \{0,1,\dots,n\} \\ &a_{i,1} = f[x_0,x_1,\dots,x_i;y_0,y_1] \;\; pentru \;\;\; i \in \{0,1,\dots,n-1\} \\ &\qquad \vdots \\ &a_{i,n-1} = f[x_0,\, x_1,\dots,x_i;y_0,y_1,\dots,y_{n-1}] \;\; pentru \;\;\; i \in \{0,1\} \\ &a_{0,n} = f[x_0;\; y_0,y_1,\dots,y_n] \;\; pentru \;\;\; i \in \{0,1,\dots,n\} \end{aligned}$$

So we obtain:

$$a_{0,0} = f[x_0; y_0] = f(x_0, y_0) = 0,$$
$$a_{1,0} = f[x_0, x_1; y_0] = \frac{f[x_1, y_0] - f[x_0, y_0]}{x_1 - x_0} = \frac{-38-0}{1-0} = -38,$$
$$a_{0,1} = f[x_0; y_0, y_1] = \frac{f[x_0, y_1] - f[x_0, y_0]}{y_1 - y_0} = -38,$$
$$a_{1,1} = f[x_0, x_1; y_0, y_1] = \frac{f[x_0, x_1; y_1] - f[x_0, x_1; y_0]}{y_1 - y_0}$$
$$= \frac{\frac{f[x_1, y_1] - f[x_0, y_1]}{x_1 - x_0} - \frac{f[x_1, y_0] - f[x_0, y_0]}{x_1 - x_0}}{y_1 - y_0} = 108.$$

Thus, $P_n(x, y) = -38(x - 0) - 38(y - 0) + 108(x - 0)(y - 0)$ $= 108xy - 38x - 38y$.

If we connect a cycle graph with $n \geq 3$ vertices to a path with k vertices by a bridge, a graph called a Tadpole graph ($T(n, k)$) is created.

Theorem 3.2: *If* $T(n, k)$ *be a Tadpole graph***,** *then*

$$F\big(T(n, k)\big) = 16n + 16k + 50.$$

Proof: The sequence of F-index values for $[n, k] = [0,0], [0,1], [1,0], [1,1]$ is as follows:

$$F(T[0,0]) = 50, \qquad F(T[0,1]) = 66,$$
$$F(T[1,0]) = 66, \qquad F(T[1,1]) = 82.$$

We obtain,

$$a_{0,0} = 50, \quad a_{1,0} = 16, \quad a_{0,1} = 16, \quad a_{1,1} = 0.$$

Hence,

$$P_n(x, y) = 50 + 16(x - 0) + 16(y - 0) = 50 + 16x + 16y. \blacksquare$$

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