Indian Journal of Science and Technology, Vol 9(4), DOI: 10.17485/ijst/2016/v9i4/77268, January 2016
ISSN (Print) : 0974-6846
ISSN (Online) : 0974-5645

Topological Indices and Interpolation of Sequences

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Abstract

In this paper, some topological indices of benzenoid graphs and mathematical graphs are computed, using the interpolation of sequences.

Keywords: Graph, Interpolation, Sequence, Topological Index

1. Introduction

Throughout this paper all graphs are assumed to be simple, finite and connected. A topological index in the chemical literature, is a function τ from the class of connected graphs into real numbers with the property that $\tau(G) = \tau(H)$ whenever G and H are isomorphic[1]. The eccentric connectivity index of a graph G, ξ^C was proposed by Sharma, Goswami and Madan[2]. This is a topological index which is defined as:

$$\xi^C(G) = \sum_{u\in V(G)} \deg(u).ecc(u)$$

where $deg(u)$ denotes the degree of the vertex u in G and $ecc(u) = Max\{d(x,u) \mid x \in V(G)\}$. The quantity $ecc(u)$ is usually named the eccentricity of vertex u in G. The minimum and maximum of eccentricity among vertices of G are called the radius and diameter of G, respectively. We encourage to interested readers to consult papers[3–10] for chemical meaning and[11] for mathematical properties of this topological index. Also for a simple and connected graph G, other topological indices, modified eccentricity connectivity Λ, edge eccentric connectivity index ξ_e^C, modified edge eccentric connectivity index $\Lambda_e(G)$, and wiener index $W(G)$ are defined as following equations respectively:

$$\Lambda(G) = \sum_{u\in V(G)} S(u).ecc(u), \quad \xi_e^C(G) = \sum_{f\in E(G)} \deg(f).ecc(f)$$

$$\Lambda_e(G) = \sum_{f\in E(G)} S(f).ecc(f), \quad W(G) = \sum_{u,v\in V(G)} d(u,v)$$

In these definitions $S(u) = \sum_{v\in N(u)} \deg(v)$, where $N(u)$ is the set of all neighborhoods of vertex u in G and also, $d(u,v)$ denote the distance between vertices u and v, in G.

For most of topological indices, a polynomial called topological polynomial is defined, so that the first derivative of such polynomial at $x = 1$ is equal to topological index. The topological polynomials corresponding to the above indices are as follows respectively:

$$ECP(G,x) = \sum_{u\in V(G)} \deg(u)\,x^{ecc(u)}, \quad \Lambda(G,x) = \sum_{u\in V(G)} S(u).x^{ecc(u)}$$

$$ECP_e(G,x) = \sum_{f\in E(G)} \deg(f).x^{ecc(f)}, \quad \Lambda_e P(G,x) = \sum_{f\in E(G)} s(f).x^{ecc(f)}$$

$$WP(G,x) = \sum_{u,v\in V(G)} x^{d(u,v)}$$

These polynomials give more information about the structure of the molecular graphs. For more

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information[12–14] are recommended. For more information about wiener index[15] is recommended.

2. The Method

The method in this paper is a kind of interpolation. For more information about interpolation and other applications in details[16–20] are purposed.

For a function f, defined on the line of real numbers, difference operator Δ is defined as $\Delta f(x) = f(x + 1) - f(x)$. For each natural number, by $\Delta^0 f = I(f) = f$ and $\Delta^n f = \Delta^{n-1}(\Delta f)$, powers of Δ is defined inductively. One of the interesting features of a polynomial is that, if the degree of polynomial $f(x)$ is n, then we have $\Delta^{n+1} f = 0$. This enables us to calculate many topological indices for infinite families of graphs, which have a common form. The following lemma is proved in[21].

Lemma 2.1

For a real value function f, $\Delta^n f = 0$, if and only if, $f(x)=a_0(x) + a_1(x)x + \dots + a_n(x)x^n$, so that, $a_0, a_1, \dots, a_n$, are all 1-periodic functions.

If for a sequence of real numbers, such as $A = \{a_n\}_{n\geq 1}$, we define, $\Delta A = \{a_{n+1} - a_n\}_{n\geq 1}$, then according to the above Lemma it can be concluded that the generator of sequence is a polynomial of degree k, if and only if $\Delta^k(A)$ is a fixed sequence while $\Delta^{k-1}A$ is not a fixed sequence. Also for an independent proof for this fact see[22].

According to the above issues, it is concluded that having some of the first values of indices, is enough to obtain a closed formula for a topological index in a family of graphs which has a common form, where the closed formula is a polynomial or a function of polynomials. To determine this closed formula which is in the form of a polynomial, it is enough to obtain differences sequences several times as far as the fixed sequence is obtained. If such a fixed sequence is not achieved, it will be concluded that the closed formula is not in a form of polynomial.

In this section, the methods to obtain closed formula in the form of polynomial, which is the generator of a sequence of real numbers such as $A = \{a_n\}_{n\geq 1}$ are introduced. Then, several topological indices will be calculated using this method.

For each real number x and each positive integer n, the falling power $x^{\underline{n}}$ is defined as $x^{\underline{n}} = x(x-1)\dots(x-n+1)$ and $x^{\underline{0}} = 1$. It is supposed that the generator of sequence of real numbers $A = \{a_n\}_{n\geq 1}$ is a polynomial of degree k, such as $P(x)$. The relation, $\Delta x^{\underline{n}} = n x^{\underline{n-1}}$, for all positive integer n is simply as certainable[23]. It is quite similar to the power derivative formula. Therefore, considering this relation as reverse, a kind of integration will be achieved to obtain the generator of a sequence in the form of polynomial. Indeed, $\Delta^{-1} x^{\underline{n}} = \frac{\mathrm{x}^{\underline{n+1}}}{\mathrm{n}+1} + \mathrm{C}$. The following example indicates that method of obtaining the generator of a sequence in the form of polynomial.

Example 2.2

Suppose that, the sequence, $A = \{a_n\}_{n\geq 1}$ in order, is listed by following sentences:

$$A = \{3, 6, 11, 18, 27, \dots\}$$

According to these sentences, we have:

$$\Delta A = \{3, 5, 7, 9 \dots\}$$

$$\Delta^2 A = \{2, 2, 2, 2 \dots\}$$

Given the above subjects, the generator of sequence is a quadratic polynomial. Using the integration on $\Delta^2 A = \{2\}_{n\geq 1}$, $\Delta A = \{2n^{\underline{1}} + C_1\}_{n\geq 1}$, will be obtained. Given the fact that the first term of ΔA, is equal to 3, it is obvious that C_1=1. Therefore, we get, $\Delta A = \{2n^{\underline{1}} + 1\}_{n\geq 1}$. The integration is repeated once more. Given the fact that the first term of sequence is equal to 3, we get $A = \{n^{\underline{2}} + n^{\underline{1}} + 2\}_{n\geq 1}$

In the next section some topological indices will be calculate via this method.

3. Main Results

The edge eccentric connectivity and the modified edge eccentric connectivity indices of benzenoid graphs will be calculated.

The benzenoid graphs consist of interconnected hexagons as a finite line shown by $L_n(G)$ where n indicates the number of hexagons in each row and column [See Figure 1].

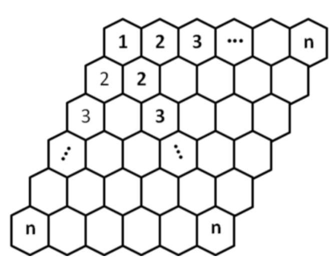

Figure 1. Symmetric benzenoid graph.

Now, in the following theorem, the edge connectivity eccentric index, $L_n(G)$ is calculated.

Theorem 3.1

The edge eccentric connectivity index, for $L_n(G)$ is equal to $.\xi_e^c\left(L_n(G)\right) = 32n^3 - 44n + 40$

Proof

The sequence of index values for *n=1,2,3,…,9,10* is as follows:

A={28,208,772,1912,3820,6688,10708,16072,22972,31600,…}

Difference sequences are as follows:

DA={180,564,1140,1908,2868,4020,5364,6900,8628,…}

D^2A ={384,576,768,960,1152,1344,1536,1728,…}

$$D^3A=\{192\}_{n\geq 1}$$

As it was seen, the generator of the sequence should be a third-degree polynomial. The integral of both sides of equation $D^3A=\{192\}_{n\geq 1}$ is calculated as. $D^2A=\left\{192n^1+C_1\right\}_{n\geq 1}$ Using the first term of D^2A, we get, C_1 = 384, and therefore $D^2A=\left\{192n^1+384\right\}_{n\geq 1}$ Again, taking the integration of both sides of equation, the following equation is obtained:

$$DA=\left\{96n^2+384n^1+180\right\}_{n\geq 1}$$

The fixed value *180* is obtained using the first value of DA. As it was expected, we have

$$A=\left\{32n^3+192n^2+180n^1+28\right\}_{n\geq 1}=\left\{32n^3-44n+40\right\}_{n\geq 1}$$

as required.

In the following theorem, the modified edge connectivity eccentric index for $L_n(G)$ is calculated.

Theorem 3.2

The modified edge eccentric connectivity index of $L_n(G)$ is obtained by following equation:

$$\Lambda_e\left(L_n(G)\right)=128n^3-72n^2-120n+140\ .$$

Proof

The sequence of index values for *n=1,2,3,…,9* is as follows:

A={76,636,2588,6700,13740,24476,39676,60108,86540,…}

Difference sequences is as follows:

DA = {560,1952,4112,7040,10736,15200,20432,26432,…}

D^2A ={1392,2160,2928,3696,4464,5232,6000,…}

$$D^3A=\{768\}_{n\geq 1}$$

As it was seen, the generator of the sequence should be a third-degree polynomial. = DA Taking integration over both sides of equation $D^3A=\{768\}_{n\geq 1}$, we get $D^2A=\left\{768n^1+1392\right\}_{n\geq 1}$. Again, using the integration of both sides of equation, the following equation is obtained:

$$DA=\left\{384n^2+1392n^1+560\right\}_{n\geq 1}$$

The fixed value, *560* is obtained by using the first value of DA. As it was expected, we get

$$A=\left\{128n^3+696n^2+560n^1+76\right\}_{n\geq 1}=\left\{128n^3-72n^2-120n+140\right\}_{n\geq 1}$$

as the result of integration, and proof is completed.

A sequence of simple triangular graphs is shown [See Figure 2].

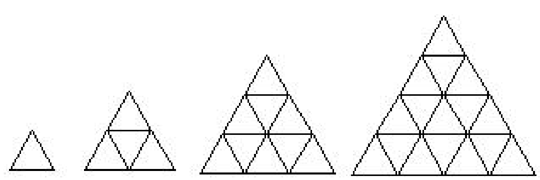

Figure 2. Triangular graphs G_n , (n=2,3,4,5)

As it can be seen, the graph G_n has $1+2+...+(n+1)=\dfrac{(n+1)(n+2)}{2}$ vertex and consists of n^2 triangle which are enclosed within a larger triangle. Now, the wiener index will be calculated for this infinite family of graphs.

Theorem 3.3

For each integer, $k\geq 0$,

$$W\left(G_{k+1}\right)=\frac{1}{40}\left[2k^5+15k^4+40k^3+45k^2+18k\right]$$

Proof

Calculating the first nine values of wiener index, the following sequence is obtained:

$A=\{0,3,21,81,231,564,1134,2142,3762\}$

Therefore, difference sequences are as follows:

$DA = \{3,18,60,150,315,588,1008,1620,\ldots\}$

$D^2A = \{15,42,90,165,273,420,612,\ldots\}$

$D^3A = \{27,48,75,108,147,192,\ldots\}$

$D^4A = \{21,27,33,39,45,\ldots\}$

$D^5A = \{6\}_{n\geq 0}$

According to these sequences, the generator of A is a fifth-degree polynomial. Calculating the integral of $D^5A=\{6\}_{k\geq 0}$, $D^4A=\left\{6k^1+21\right\}_{k\geq 0}$ is obtained. Consecutive calculating of integral,

$$D^3A=\left\{3k^2+21k^1+27\right\}_{k\geq 0},$$

$$D^2A=\left\{k^3+\frac{21}{2}k^2+27k^1+15\right\}_{k\geq 0}$$

$$DA=\left\{\frac{1}{4}k^4+\frac{7}{2}k^3+\frac{27}{2}k^2+15k^1+3\right\}_{k\geq 0}$$

And

$$A=\frac{1}{40}\left\{\frac{1}{20}k^5+\frac{7}{8}k^4+\frac{9}{2}k^3+\frac{15}{2}k^2+3k^1\right\}_{k\geq 0}$$
$$=\left\{\frac{1}{40}(2k^5+15k^4+40k^3+45k^2+18k)\right\}_{k\geq 0}$$

are obtained, as expected.

4. Conclusion

Whenever the closed formula of a topological index of an infinite family of graphs is in the form of a polynomial, the degree of polynomial as well as the polynomial itself can be calculated using the successive difference method.

5. References

1. Hosoya H. Topological index, a newly proposed quantity characterizing the topological nature of structure isomers of saturated hydrocarbons. Bull Chem Soc Japan. (1971); 44(1971):2332–9.
2. Sharma V, Goswami R, Madan AK. Eccentric connectivity index: A novel highly discriminating topological descriptor for structure-property and structure-activity studies. J Chem Inf Comput Sci. 1997; 37(2):273–82.
3. Ashrafi AR, Saheli M, Ghorbani M. The eccentric connectivity index of nanotubes and nanotori. J Comput Appl Math. 2010; 235(16):4561–6.
4. Ashrafi AR, Ghorbani M, Jalali M. Eccentric connectivity polynomial of an infinite family of fullerenes. Optoelectron Adv Mater Rapid Comm. (2009); 3(8):823–6.
5. Ashrafi AR, Ghorbani M. Distance matrix and diameter of two infinite family of fullerenes. Optoelectron Adv Mater Rapid Comm. 2009; 3(6):596–9.
6. Dureja H, Madan AK. Super augmented eccentric connectivity indices: New-generation highly discriminating topological descriptors for QSAR/QSPR modeling. Med Chem Res. 2007; 16(2007):331–41.
7. Ghorbani M, Ashrafi AR, Hemmasi M. Eccentric connectivity polynomials of fullerenes. Optoelectron Adv Mater – Rapid Comm. 2009; 3(12):1306–8.
8. Gupta S, Singh M, Madan AK. Application of graph theory: Relationship of eccentric connectivity index and wiener index with anti inflammatory activity. J Math Anal Appl. 2002; 266(2):259–68.
9. Kumar V, Sardana, S, Madan AK. Predicting anti-HIV activity of 2,3-diary l-1,3-thiazolidin-4-ones: Computational approaches using reformed eccentric connectivity index. J Mol Model. 2004; 10(2004):399–407.
10. Sardana S, Madan AK. Application of graph theory: Relationship of molecular connectivity index, Wiener index and eccentric connectivity index with diuretic activity. Match Commun Math Comput Chem. 2001; 43(43):85–98.
11. Zhou B, Du Z. On eccentric connectivity index. Match Commun Math Comput Chem. 2010; 63(2010):181–98.
12. Diudea MV, Ivanciuc O, Nikolic S, Trinajstic N. Matrices of reciprocal distance. polynomials and derived numbers. J Match Commun Math Comput Chem. 1997; 35(1997):41–64.
13. Graham RL, Lovasz L. Distance Matrix Polynomials of Trees. AdV. Math. (1978); 29(1978) :60-88.
14. Imrich W, Klavzar S. Product graphs: Structure and recognition. New York, USA: John Wiley and Sons; 2000.

15. Gutman I, Kortevlyesi T. Wiener indices and molecular surfaces. Z Naturforsch. 1995; 50(7):669–71.
16. Ahmad RH, Majid R. The fractional cubic spline interpolation without using the derivative values. Indian Journal of Science and Technology. 2012; 5(10):3433–9.
17. Muthu LAC, Santhi HM. Estimation of surface runoff potential using SCS-CN method integrated with GIS. Indian Journal of Science and Technology. 2015; 8(28):1–5.
18. Omar Z, Kuboye JO. Derivation of block methods for solving second order ordinary differential equations directly using direct integration and collocation approaches. Indian Journal of Science and Technology. 2015; 8(12):1–4.
19. Sergienko IV, Lytvyn ON, Lytvyn OO, Mezhuyev VI, Lobanova LS, Zalyzhna GV. The numerical implementation of the linear integro differential equations method for the solution of non-stationary heat conduction problem with two space variables. Indian Journal of Science and Technology. 2015; 8(30):1–7.
20. Hamidreza M, Fazel H. Weights guaranteeing polefree barycentric rational interpolation. Indian Journal of Science and Technology. 2013; 6(11):5450–8.
21. Paulo N, Jorge S. Berkeley Problems in Mathematics. Springer; 1998.
22. Alaeiyan M, Ebrahimi M. New method for computing some topological indices. J Computational and Theoretical Nanoscience. 2015; 12(10):1–4.
23. Kunin GB. The finite difference calculus and applications to the interpolation of sequences. MIT Undergraduate Journal of Mathematics. 2001; 232(2001):101–9.