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Interpolation Method and Topological Indices: The case of Fullerenes C_{12k+4}

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Abstract

Polynomial interpolation can be used to obtain closed formulas for topological indices of infinite series of molecular graphs. The method is discussed and its advantages and limitations are pointed out. This is illustrated on fullerenes C_{12k+4} and four topological indices: the Wiener index, the edge Wiener index, the eccentric connectivity index, and the reverse Wiener index. The results for the edge Wiener index correct earlier computations from the literature. Related formulas are derived for cyclic phenylenes.

1 Introduction

Computations of topological indices and deriving related closed formulas lie in the very center of chemical graph theory. Different methods and algorithms have been developed for this sake. An optimal case is when a closed formula can be deduced, because in that case the invariant in question can in principle be computed in constant time. A useful approach to obtain formulas is the so-called interpolation method [6, 7]. In the literature it is typically used without proper mathematical background and the obtained formulas are taken as granted despite the fact that they are eventually not rigorously proved. The purpose of this paper is to point out how the method should be used and to provide its further applications. Along the way we also point out an error from the literature and correct it.

Topological indices are numerical parameters related to the molecular structure and are used in the study of biological activities and physico-chemical properties of molecular graphs. Numerous such indices are based on the distance function of a graph. The first (distance based) topological index is the Wiener index [21]. It has found considerable applications in QSPR and QSAR [9, 18, 20] and is still extensively investigated [4, 8, 10, 16, 22, 23].

The other three distance based topological indices we will consider are the reverse Wiener index introduced by Balaban et al. [19], the eccentric connectivity index introduced by Sharma et al. [3], and the edge Wiener index introduced in [14]. The study of the latter index can be reduced to the study of the Wiener index of line graphs [8, 22]. The cut method [15] for the edge Wiener index was developed in [24]. The eccentric connectivity index is very extensively studied in these years, [2, 11, 17] is just a sample of recent investigations. For some more results on the reverse Wiener index see [5, 12].

The paper is organized as follows. In the rest of this section we recall definitions of the four topological that are of interest here. Then, in the subsequent section, the interpolation method is described and requirements that need to be fulfilled in order to apply the method are emphasized. In Section 3, the method is applied to obtain closed formulas for four topological indices of fullerenes C_{12k+4}. We conclude the paper by giving related formulas for cyclic phenylenes.

Let G be a connected graph, then the *distance* between vertices u and v is denoted by $d(u, v)$. The *diameter* of G is the maximum distance between its vertices and denoted $\mathrm{diam}(G)$. The *eccentricity* $\mathrm{ecc}(u)$ of u is the maximum distance between u and any other vertex of G. The distance between edges $g = u_1v_1$ and $f = u_2v_2$ is defined as

$$d_e(g, f) = \min\{d(u_1, u_2), d(u_1, v_2), d(v_1, u_2), d(v_1, v_2) \;\; + 1\,.$$

Equivalently, this is the distance between the vertices g and f in the line graph of G [14]. The degree of u will be denoted $\deg(u)$.

Let G be a connected graph on n vertices. Then the *Wiener index* $W(G)$, the *edge Wiener index* $W_e(G)$, the *reverse Wiener index* $RW(G)$, and the *eccentric connectivity index* $\xi(G)$, are respectively defined as follows:

$$\begin{aligned} W(G) &= \sum_{\{u,v\}\in\binom{V(G)}{2}} d(u,v)\,, \\ W_e(G) &= \sum_{\{f,g\}\in\binom{E(G)}{2}} d_e(f,g)\,, \\ RW(G) &= \frac{1}{2}n(n-1)\mathrm{diam}(G) - W(G)\,, \\ \xi(G) &= \sum_{u\in V(G)} \mathrm{ecc}(u)\mathrm{deg}(u)\,. \end{aligned}$$

2 Interpolation method

Let $\{G_k\}_{k\geq 1}$ be a series of graphs and let I be a topological index. Suppose that there exists $n_0 \in \mathbb{N}$ such that for any $n \geq n_0$, $I(G_n) = p(n)$, where p is a polynomial of degree r. Then p can be determined by interpolating the values $I(G_{n_0}), I(G_{n_0+1}), \ldots, I(G_{n_0+r})$. We will say that p *interpolates* I *on* $\{G_k\}_{k\geq 1}$. Consequently, for any i, $I(G_i)$ can be determined in constant time from the list of initial values $I(G_k)$, $1 \leq k < n_0$, and the polynomial p.

To apply the interpolation method efficiently, it is important to give a bound on the degree of the polynomial p. For this sake, the following observation is useful:

Lemma 2.1 *Suppose that* p *interpolates* I *on* $\{G_k\}_{k\geq 1}$. *If there exists a positive constant* α *such that* $I(G_k) < \alpha k^r$, *then* $\deg(p) \leq r$.

Proof. Suppose on the contrary that $\deg(p) > r$. Then $\frac{I(G_k)}{p(k)} < \frac{\alpha k^r}{p(k)} \xrightarrow[k\to\infty]{} 0$. But this is not possible because p interpolates I on $\{G_k\}_{k\geq 1}$ and hence there exists $n_0 \in \mathbb{N}$ such that for any $n \geq n_0$, $I(G_n) = p(n)$, and consequently $\frac{I(G_k)}{p(k)} \xrightarrow[k\to\infty]{} 1$. □

In order to apply the interpolation method, the following requirements must be fulfilled:

1. Initial deviations should be ruled out, that is, the smallest n_0 has to be determined such that the interpolation works for all $n \geq n_0$.

2. It has to be proved that $I(G_n)$ is a **fixed** polynomial function, that is, there exists a polynomial p such that $I(G_n) = p(n)$ holds for **any** $n \geq n_0$.

3. A constant upper bound on the degree of p must be given.

Out of these three conditions, the second one seems to be most difficult to fulfill and we know of no example where it was done. Hence all the corresponding theorems stated in the literature are only conditionally true! On the other hand, if an obtained formula has been verified for large enough $n \geq n_0$, then the obtained formula can be safely used in practice.

After the above three conditions are fulfilled, the interpolation is straightforward. Suppose $\deg(p) \leq r$, then by interpolating the points $(n_0, I(G_{n_0})), (n_1, I(G_{n_1})), \ldots, (n_0 + r, I(G_{n_0+r}))$, a closed formula (a polynomial) is obtained. This follows from the well-known fact that if $f(x)$ and $g(x)$ are polynomials of degrees m and n, $m \leq n$, and have more than n points in common, then $f(x) = g(x)$.

3 Fullerenes C_{12k+4}

In this section we demonstrate the use of the interpolation method on the fullerene graphs C_{12k+4}. These fullerenes, whose definition should be clear from Fig. 1, were studied for instance in [1, 13].

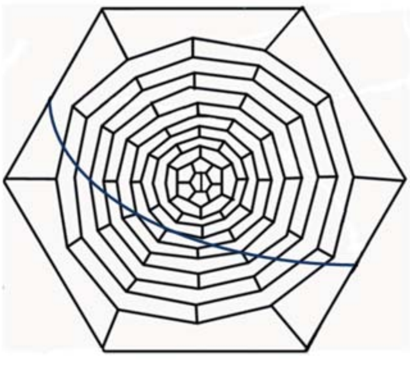

Figure 1: C_{12k+4}, $k = 12$

The paper [13] brings values for the (first and the second) edge Wiener index of these fullerenes and interpolates it by polynomial of degree 12. However the reported results appear to be wrong as it will be justified later. A particular motivation for the present paper is thus also to fill this gap. We begin with the Wiener index and first bound the degree of a possible interpolation polynomial:

Lemma 3.1 *Suppose p interpolates W on $\{C_{12k+4}\}_{k\geq 3}$. Then p is a cubic polynomial.*

Proof. Clearly, if G is a connected graph on n vertices, then $W(G) \leq \binom{n}{2}\mathrm{diam}(G)$. (Moreover, the equality holds here if and only if G is a complete graph.) Since $\mathrm{diam}(C_{12k+4}) = 2k-1$ holds for $k \geq 7$, it follows that $W(C_{12k+4}) \leq \binom{12k-8}{2}(2k-1) = 144k^3 - 276k^2 + 174k - 36$, $k \geq 7$. The assertion now follows from Lemma 2.1. □

Using Lemma 3.1, the interpolation method is now applied by interpolating four consecutive points but having in mind that initial deviations should be ruled out. It turns out that the values $W(C_{12k+4})$, $3 \leq k \leq 6$, are sporadic. The values were computed up to $k = 100$, see Table 1, so that the exact statement is:

Theorem 3.2 $W(C_{28}) = 1198$*,* $W(C_{40}) = 3004$*,* $W(C_{52}) = 5894$*,* $W(C_{64}) = 10092$*, and for* $7 \leq k \leq 100$*,* $W(C_{12k+4}) = 48k^3 - 96^2 + 908k - 2274$.

Since the interpolation works for $7 \leq k \leq 100$ it is very likely that if holds for all k and hence the obtained formula can be therefore used for all practical purposes. However, one would still need to prove that $I(G_k)$ is a fixed polynomial function.

In Table 1 values for the other three indices of interest here are also given.

We continue with the edge Wiener index of C_{12k+4} which is equal to $W(L(C_{12k+4}))$, where $L(G)$ denotes the line graph of G. Since $|L(C_{12k+4})| = 18k - 12$ and $\mathrm{diam}(L(C_{12k+4})) \leq \mathrm{diam}(C_{12k+4}) + 1 = 2k$, we infer that an interpolation polynomial for the edge Wiener index of C_{12k+4} is again cubic. In particular, $W_e(C_{12k+4}) \leq \binom{18k-12}{2}2k$. Since the computed numbers from [13] are larger than this estimate, the results obtained there are not correct. The interpolation does not work for $k \leq 6$, but for $7 \leq k \leq 100$ we have:

$$W_e(C_{12k+4}) = 108k^3 - 216k^2 + 2199k - 5457\,.$$

For the reverse Wiener index of C_{12k+4} we have for $7 \leq k \leq 100$:

$$RW(C_{12k+4}) = 96k^3 - 180k^2 - 734k + 2238\,.$$

Finally, for the eccentric connectivity index an interpolation polynomial, if it exists, is quadratic. Indeed, this follows because for each vertex v of C_{12k+4}, we have $\deg(v) = 3$

k	Wiener	edge Wiener	reverse Wiener	ecc. connectivity
3	1198	2870	1070	468
4	3004	7067	3236	852
5	5894	13708	6040	1236
6	10092	23299	12084	1716
7	15842	36396	21208	2280
8	23422	53607	33998	2988
9	33114	75570	51036	3804
10	45206	102933	72898	4764
11	59986	136344	100160	5832
12	77742	176451	133398	7008
13	98762	223902	173188	8292
14	123334	279345	220106	9684
15	151746	343428	274728	11184
16	184286	416799	337630	12792
17	221242	500106	409388	14508
18	262902	593997	490578	16332
19	309554	699120	581776	18264
20	361486	816123	683558	20304
⋮	⋮	⋮	⋮	⋮
100	47128526	106054443	94128838	533424

Table 1: The topological indices of C_{12k+4} fullerene

and $\mathrm{ecc}(v) \leq \mathrm{diam}(C_{12k+4}) = 2k-1$, $k \geq 7$. On the other hand it interestingly turned out that the interpolation starts working from $k \geq 9$, so that for $9 \leq k \leq 100$ we can state:

$$\xi(C_{12k+4}) = 54k^2 - 66k + 24\,.$$

4 Cyclic phenylenes

Cyclic phenylenes were studied among others in [7, 25]. The cyclic phenylene R_h is defined for any $h \geq 3$, its definition should be clear from the example of R_5 depicted in Fig. 2.

In this case the interpolation method works for all the four indices for any $h \geq 3$ except for the eccentric connectivity index for which $h = 3$ is an exception. The obtained results for $h \leq 100$ are:

$$\begin{aligned} W(R_h) &= 9h^3 + 36h^2 - 36h\,, \\ W_e(R_h) &= 16h^3 + 56h^2 - 45h\,, \\ RW(R_h) &= 9h^3 + 33h^2 + 24h\,, \\ \xi(R_h) &= \begin{cases} 270, & h = 3; \\ 16h^2 + 46h, & h \geq 4. \end{cases} \end{aligned}$$

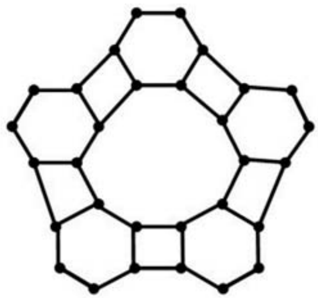

Figure 2: The cyclic phenylene R_5

The expression for $W(R_h)$ was earlier reported in [7].

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