SOLUTIONS FOR TWO CONJECTURES ON THE INVERSE PROBLEM OF THE WIENER INDEX OF PEPTOIDS*

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Abstract. In this paper, we give solutions for the two conjectures on the inverse problem of the Wiener index of peptoids proposed by Goldman et al. We give the first conjecture a positive proof and the second conjecture a negative answer.

Key words. combinatorial chemistry, Wiener index, peptoid

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1. Introduction. In drug design and molecular recognition, combinatorial chemistry has played a powerful role in recent years. One of the central problems is the construction of a molecular graph with given chemical or physical properties. A chemical or physical property can be quantitatively represented by some topological index [1]. The problem here is to find a molecular graph with a given value of some topological index. In [1], the authors studied the problem for the Wiener index. They proposed two conjectures related to the so-called *inverse problem of peptoids*. A peptoid is represented by a large molecular graph constructed from some pieces of given small molecular graphs by joining them in a linear scaffold way, i.e., chaining them linearly. The problem is to find a peptoid with these given small pieces as fragments such that it has the desired Wiener index value. The ordering or arrangement of these pieces in a peptoid determines the value of the Wiener index. The two conjectures are to determine the orderings or arrangements under which the values are minimum or maximum. As one can see in the statements of the conjectures, the optimal problems are purely mathematical. We can go without any notation or terminology on graph theory or chemistry.

Let n_1, n_2, \ldots, n_N be N positive integers; define

$$D = \sum_{i=1}^{N} \sum_{j=i+1}^{N} (j-i)n_i n_j$$

For an ordering or rearrangement $\pi = \pi(1)\pi(2)\ldots\pi(N)$ of $1, 2, \ldots, N$, define

$$D(\pi) = \sum_{i=1}^{N} \sum_{j=i+1}^{N} (j-i)n_{\pi(i)}n_{\pi(j)}.$$

Conjecture 5.1 of [1] is stated as follows.

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CONJECTURE 1. Given $n_1 \leq n_2 \leq \cdots \leq n_N$, the ordering for the minimum value of D is

$$\pi_{\min}(i) = \begin{cases} 2i-1 & \text{if } i \le \frac{N}{2} \\ 2(N-i+1) & \text{if } i > \frac{N}{2}. \end{cases}$$

Conjecture 5.2 of [1] is stated as follows.

CONJECTURE 2. An algorithm to compute the ordering for the maximum value of D, given $n_1 \leq n_2 \leq \cdots \leq n_N$, is as follows:

$$\begin{split} L_P &= 1; L = 0\\ R_p &= N; R = 0\\ For \ i &= N \ down \ to \ 1 \ do\\ if \ R &\geq L, \ then\\ \pi_{max}(L_p) &= i; L_p = L_p + 1; L = L + n_i;\\ else\\ \pi_{max}(R_p) &= i; R_p = R_p - 1; R = R + n_i. \end{split}$$

We solve these two conjectures in the following sections. In section 2, we do some preparations by introducing two inequalities due to Hardy, Littlewood, and Pólya [2] and Wiener [4], respectively. In section 3, we prove Conjecture 1 vigorously by using Hardy, Littlewood, and Pólya's inequality. In section 4, we show that Conjecture 2 is not correct. The algorithm in Conjecture 2 does not always give the maximum value. We give a better upper bound for the maximum value by using Wiener's inequality. Finally, in section 5, we analyze the difficulty in finding the exact ordering to attain the maximum value.

2. Preliminaries. We follow the notations of [2] or [3]. Suppose that we are given a set of a finite number of nonnegative numbers x_1, x_2, \ldots, x_N , or x_{-n}, \ldots, x_{-1} , x_0, x_1, \ldots, x_n , denoted by (x). An ordering or rearrangement of them is x'_1, x'_2, \ldots, x'_N , or $x'_{-n}, \ldots, x'_{-1}, x'_0, x'_1, \ldots, x'_n$, denoted by (x'), where $\{x'_1, x'_2, \ldots, x'_N\} = \{x_1, x_2, \ldots, x_N\}$ and $\{x'_{-n}, \ldots, x'_{-1}, x'_0, x'_1, \ldots, x'_n\} = \{x_{-n}, \ldots, x_{-1}, x_0, x_1, \ldots, x_n\}$. Some special orderings are given as follows:

$$(\bar{x}) = \bar{x}_1 \le \bar{x}_2 \le \dots \le \bar{x}_N$$

or

$$(\bar{x}) = \bar{x}_{-n} \le \dots \le \bar{x}_{-1} \le \bar{x}_0 \le \bar{x}_1 \le \dots \le \bar{x}_n,$$

i.e., increasing ordering.

$$(x^+) = x_0^+ \ge x_1^+ \ge x_{-1}^+ \ge x_2^+ \ge x_{-2}^+ \ge \cdots$$

and

$$(^+x) = ^+ x_0 \ge ^+ x_{-1} \ge ^+ x_1 \ge ^+ x_{-2} \ge ^+ x_2 \ge \cdots$$

For example, in the example of [1, p. 283], $(x) = 8, 13, 2, 17, 19, 18, 28, 5; (\bar{x}) = (n) = 2, 5, 8, 13, 17, 18, 19, 28; (x^+) = 5, 13, 18, 28, 19, 17, 8, 2, and (+x) = 2, 8, 17, 19, 28, 18, 13, 5.$

From [2] or [3], we have the following theorem.

THEOREM 2.1 (Hardy, Littlewood and Pólya). Suppose that c, x, y are nonnegative and c symmetrically decreasing so that

$$c_0 \ge c_1 = c_{-1} \ge c_2 = c_{-2} \ge \cdots \ge c_{2k} = c_{-2k},$$

while x and y are given except in arrangement. Then the bilinear form

(1)
$$S^{(1)} = \sum_{r=-k}^{k} \sum_{s=-k}^{k} c_{r-s} x_r y_s$$

attains its maximum when (x) is (x^+) and (y) is (y^+) , or (x) is (^+x) and (y) is (^+y) . From [2] or [4], we have the following theorem.

THEOREM 2.2 (Wiener). If $c_2 \ge c_3 \ge \cdots \ge c_{2n} \ge 0$ and the sets (x) and (y) are nonnegative and given except in arrangement, then

(2)
$$S^{(2)} = \sum_{r=1}^{n} \sum_{s=1}^{n} c_{r+s} x_r y_s$$

is a maximum when (x) and (y) are both in decreasing order.

It is easy to see that the two bilinear forms of (1) and (2) have the coefficient matrices

$$C^{(1)} = \begin{pmatrix} c_0 & c_1 & c_2 & c_3 & \cdots & \cdots & \cdots & \cdots \\ c_1 & c_0 & c_1 & c_2 & \cdots & \cdots & \cdots & \cdots \\ c_2 & c_1 & c_0 & c_1 & \cdots & \cdots & \cdots & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & c_1 & c_0 & c_1 \\ \cdots & \cdots & \cdots & \cdots & \cdots & c_2 & c_1 & c_0 \end{pmatrix}_{(2k+1)\times(2k+1)}$$

and

$$C^{(2)} = \begin{pmatrix} c_2 & c_3 & c_4 & c_5 & \cdots & \cdots & c_{n+1} \\ c_3 & c_4 & c_5 & \cdots & \cdots & \cdots & \cdots \\ c_4 & c_5 & \cdots & \cdots & \cdots & \cdots & \cdots \\ c_5 & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & c_{2n-2} \\ c_{n+1} & \cdots & \cdots & \cdots & c_{2n-2} & c_{2n-1} \\ c_{n+1} & \cdots & \cdots & \cdots & c_{2n-2} & c_{2n-1} \\ \end{pmatrix}_{n \times n}$$

respectively.

So, we have

$$S^{(1)} = (x_{-k}, \dots, x_{-1}, x_0, x_1, \dots, x_k) C^{(1)} \begin{pmatrix} y_{-k} \\ \vdots \\ y_{-1} \\ y_0 \\ y_1 \\ \vdots \\ y_k \end{pmatrix}$$

212

and

$$S^{(2)} = (x_1, x_2, \dots, x_n) C^{(2)} \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}.$$

3. The proof of Conjecture 1. We shall use Theorem 2.1 to prove Conjecture 1. Since Conjecture 1 is about optimal minimum, while Theorem 2.1 is about optimal maximum, we have to do some transformation in the following.

First, we note that

$$2D = \sum_{i=1}^{n} \sum_{j=1}^{n} |j - i| n_i n_j$$

with the coefficient matrix as follows:

$$A = \begin{pmatrix} 0 & 1 & 2 & \cdots & N-2 & N-1 \\ 1 & 0 & 1 & \cdots & N-3 & N-2 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ N-2 & N-3 & N-4 & \cdots & 0 & 1 \\ N-1 & N-2 & N-3 & \cdots & 1 & 0 \end{pmatrix}_{N \times N.}$$

Then,

(3)

$$D = \frac{1}{2} (n_1, n_2, \dots, n_N) A \begin{pmatrix} n_1 \\ n_2 \\ \vdots \\ n_N \end{pmatrix}.$$

Take the matrix $C^{(1)} = NI_N - A$, where I_N is the identity of order N, and consider the following bilinear (quadratic) form:

$$(n_1, n_2, \dots, n_N) C^{(1)} \begin{pmatrix} n_1 \\ n_2 \\ \vdots \\ n_N \end{pmatrix}$$
$$= (n_1, n_2, \dots, n_N) NI_N \begin{pmatrix} n_1 \\ n_2 \\ \vdots \\ n_N \end{pmatrix} - (n_1, n_2, \dots, n_N) A \begin{pmatrix} n_1 \\ n_2 \\ \vdots \\ n_N \end{pmatrix}$$
$$= N \left(\sum_{i=1}^N n_i\right)^2 - 2D.$$

Since the term $N(\sum_{i=1}^{n} n_i)^2$ in (3) is independent of the orderings of n_1, n_2, \ldots, n_N , we have that (3) reaches its optimal maximum by some ordering of n_1, n_2, \ldots, n_N if and only if D reaches its optimal minimum. Since here the matrix $C^{(1)}$ satisfies the

conditions of Theorem 2.1, we know that (3) reaches its optimal maximum when (n) is (n^+) or (+n), which is exactly the ordering given in Conjecture 1. Therefore, D reaches its optimal minimum when (n) is the ordering given in Conjecture 1. The proof is complete. \Box

4. Negative answer for Conjecture 2 and a better upper bound. We use examples to give a negative answer for Conjecture 2. The example of [1, p. 283] is shown in Table 1.

TABLE 1 The table of [1, p. 283].

i	1	2	3	4	5	6	7	8
n_i	2	5	8	13	17	18	19	28
$n_{\pi_{max}(i)}$	28	18	8	2	5	13	17	19

First, we point out that by executing the algorithm in Conjecture 2, we get a different ordering from Table 1, with the exchange of the two numerals 18 and 17 in the third line. We denote the ordering in Table 1 by π_t , not by π_{max} , and the ordering determined by the algorithm of Conjecture 2 by π_a . So $\pi_t = 8, 6, 3, 1, 2, 4, 5, 7$. In Appendix A, we show that $\pi_a = 8, 5, 3, 1, 2, 4, 6, 7$ by executing the algorithm. We do not know if this π_a gives the optimal maximum. However, we do know that $D(\pi_a) > D(\pi_t)$. In fact, we have that

$$D(\pi_t) - D(\pi_a) = (n_6 - n_5)[5(n_7 - n_8) + 3(n_4 - n_3) + (n_2 - n_1)]$$

= (18 - 17)[5(19 - 28) + 3(13 - 8) + (5 - 2)]
= 5 × (-9) + 3 × 5 + 3
= -45 + 18 = -27 < 0,

i.e., $D(\pi_a) > D(\pi_t)$.

(4)

Does this mean that the algorithm in Conjecture 2 really gives the ordering for the optimal maximum? The answer is "no." One may argue that the ordering of the numerals given in the table of [1, p. 283] is misprinted by the authors' carelessness. This is also not the case. In fact, from (4) we can see that $n_6 - n_5$ is always positive when $n_5 \neq n_6$, and so are $n_4 - n_3$ and $n_2 - n_1$. However, $n_7 - n_8$ is always negative when $n_7 \neq n_8$. One can imagine that by properly assigning the values of n_1, n_2, \ldots, n_8 , we can get $D(\pi_a) > D(\pi_t)$, as in the above example, and $D(\pi_a) < D(\pi_t)$ in some other cases. This is really the case. For example, we take $n_1 = 1$, or any number smaller than 8, $n_2 = 20$, $n_3 = 21$, $n_4 = 22$, $n_5 = 23$, $n_6 = 24$, $n_7 = 25$, $n_8 = 28$. The ordering given by π_t and the ordering π_a obtained by the algorithm of Conjecture 2 are shown in Table 2.

TABLE 2 The orderings given by π_t and π_a , respectively.

i	1	2	3	4	5	6	7	8
n_i	1	20	21	22	23	24	25	28
$n_{\pi_t(i)}$	28	24	21	1	20	22	23	25
$n_{\pi_a(i)}$	28	23	21	1	20	22	24	25

From (4), we have

$$D(\pi_t) - D(\pi_a) = (24 - 23)[5(25 - 28) + 3(22 - 21) + (20 - 1)]$$

= 5 × (-3) + 3 × 1 + 19 = 7 > 0.

i.e., $D(\pi_t) > D(\pi_a)$. In fact, since $n_6 - n_5 > 0$, from (4) we know that $D(\pi_t) > D(\pi_a)$ if $5(n_8 - n_7) < 3(n_4 - n_3) + (n_2 - n_1)$, while $D(\pi_t) < D(\pi_a)$ if $5(n_8 - n_7) > 3(n_4 - n_3) + (n_2 - n_1)$. So we can construct infinitely many examples to show that $D(\pi_t) > D(\pi_a)$ by properly assigning the values of n_1, n_2, \ldots, n_8 and also infinitely many other examples to show that $D(\pi_t) < D(\pi_a)$, the other way round. We do not know that if this $D(\pi_t)$ is the optimal maximum for these new n_i 's. However, it is greater than the value under the ordering given by the algorithm of Conjecture 2.

So the ordering with optimal maximum value is still unknown. We tried to find it but failed. First, we look at the ordering given by Conjecture 1, which attains the optimal minimum. Imagine that we have a balance, or a rod with support point at the center, and we want to hang N things with weights n_1, n_2, \ldots, n_N on it. To reach the minimum, we hang the heaviest one n_N at the (near) center, then we take turns to hang the next heaviest things to the left (or right) and right (or left) side of n_N . One may imagine that the maximum might be attained the other way round, i.e., hang the lightest one n_1 at the (near) center, then take turns to hang the next lightest things to the left (or right) and right (or left) side of n_1 . We denote this ordering by π_b . Unfortunately, for N = 8 we have that

$$D(\pi_a) - D(\pi_b) = (n_8 - n_7)[5(n_6 - n_5) + 3(n_4 - n_3) + (n_2 - n_1)] > 0$$

and

$$D(\pi_t) - D(\pi_b) = [(n_8 - n_7) + (n_6 - n_5)][3(n_4 - n_3) + (n_2 - n_1)] > 0$$

i.e.,

$$D(\pi_b) < D(\pi_a)$$
 and $D(\pi_b) < D(\pi_t)$.

So the intuitive observation does not give an ordering with the optimal maximum. Indeed, finding such an ordering is not an easy thing. This is why the authors of [1] did not give an exact ordering but instead an algorithmic ordering. The above analysis shows us that, unlike the optimal minimum case, to obtain the optimal maximum, the ordering is not purely dependent on the value-ordering of n_1, n_2, \ldots, n_N but mainly dependent on how large the values n_1, n_2, \ldots, n_N are themselves. Although to give an exact ordering for the optimal maximum is almost hopeless (see the analysis in section 5), we can give a better upper bound for the optimal maximum by Theorem 2.2, which could be much better than the upper bound $\frac{N^3-N}{6}n_N^2$ in [1] and useful in the inverse problem for peptoids. First, we note that we can rewrite D as follows:

$$D = (n_1, n_2, \dots, n_N) \begin{pmatrix} N-1 & N-2 & N-3 & \cdots & 2 & 1 & 0 \\ N-2 & N-3 & N-4 & \cdots & 1 & 0 \\ \vdots & \vdots & \vdots & \vdots & & \\ 2 & 1 & 0 & & & & \\ 1 & 0 & & & & & \\ 0 & & & & & & & \end{pmatrix} \begin{pmatrix} n_N \\ n_{N-1} \\ \vdots \\ n_2 \\ n_1 \end{pmatrix}.$$

Denote the coefficient matrix by $C^{(2)}$. Then, $C^{(2)}$ satisfies the conditions of

Theorem 2.2. Therefore, for any ordering π of $1, 2, \dots, N$, we have

$$D(\pi) \le (n_N, n_{N-1}, \dots, n_2, n_1)C^{(2)} \begin{pmatrix} n_N \\ n_{N-1} \\ \vdots \\ n_2 \\ n_1 \end{pmatrix}.$$

So, we have proved the following theorem. THEOREM 4.1.

$$D_{max} \leq (n_N, n_{N-1}, \dots, n_2, n_1) \\ \cdot \begin{pmatrix} N-1 & N-2 & N-3 & \cdots & 2 & 1 & 0 \\ N-2 & N-3 & N-4 & \cdots & 1 & 0 \\ \vdots & \vdots & \vdots & \vdots & & \\ 2 & 1 & 0 & & & \\ 1 & 0 & & & & & \\ 0 & & & & & & \end{pmatrix} \begin{pmatrix} n_N \\ n_{N-1} \\ \vdots \\ n_2 \\ n_1 \end{pmatrix}.$$

5. Difficulty analysis for finding the ordering π_{max} . From the three orderings π_t, π_a , and π_b , we observed that all of them arrange the values n_1, n_2, \ldots, n_N concavely with the valley at the (nearly) central position. Can it be true that the optimal maximum is always attained by some ordering that arranges n_1, n_2, \ldots, n_N in a concave way? The following analysis shows in some extent that the answer is "no." This negative answer shows that in some sense finding the ordering π_{max} could be very difficult.

Suppose that we have a concave ordering π for n_1, n_2, \ldots, n_N such that $\pi(i) > \pi(j)$ when $i < j \leq \lfloor \frac{N}{2} \rfloor + 1$, where $\lfloor x \rfloor$ denotes the maximum integer less than or equal to x. We construct another ordering π' from π by

$$\pi'(k) = \begin{cases} \pi(k), & k \neq i, j, \\ \pi(j), & k = i, \\ \pi(i), & k = j, \end{cases}$$

i.e., by exchanging $\pi(i)$ and $\pi(j)$ and keeping the others unchanged. Then, π' is no longer a concave ordering for n_1, n_2, \ldots, n_N . We shall show that sometimes $D(\pi) > D(\pi')$ and sometimes $D(\pi) < D(\pi')$, the other way round. First, by careful calculation, we can obtain that

$$D(\pi') - D(\pi) = \sum_{k=1}^{i-1} (j-i)n_{\pi(k)}(n_{\pi(i)} - n_{\pi(j)}) + \sum_{k=i+1}^{j-1} (2k - (i+j))n_{\pi(k)}(n_{\pi(j)} - n_{\pi(i)}) + \sum_{k=j+1}^{N} (j-i)n_{\pi(k)}(n_{\pi(j)} - n_{\pi(i)}) = (n_{\pi(j)} - n_{\pi(i)}) \sum_{k=1, k \neq i, j}^{N} \alpha_k n_{\pi(k)},$$

where

$$\alpha_k = \begin{cases} j-i, & k = 1, 2, \dots, i-1, \\ (i+j)-2k, & k = i+1, \dots, j-1, \\ -(j-i), & k = j+1, \dots, N. \end{cases}$$

Note that $n_{\pi(i)} - n_{\pi(j)} > 0$ by our assumption that $n_{\pi(i)} > n_{\pi(j)}$. Example 5.1. When j = i + 1, we have

$$\frac{D(\pi') - D(\pi)}{n_{\pi(i)} - n_{\pi(i+1)}} = n_{(\pi(1)} + n_{\pi(2)} + \dots + n_{\pi(i-1)}) - (n_{\pi(i+2)} + n_{\pi(i+3)} + \dots + n_{\pi(N)}).$$

Example 5.2. When j = i + 2, we have

$$\frac{D(\pi') - D(\pi)}{n_{\pi(i)} - n_{\pi(i+2)}} = 2n_{\pi(1)} + 2n_{\pi(2)} + \dots + 2n_{\pi(i-1)} - 2n_{\pi(i+3)} - 2n_{\pi(i+4)} - \dots - 2n_{\pi(N)} = 2[(n_{\pi(1)} + n_{\pi(2)} + \dots + n_{\pi(i-1)}) - (n_{\pi(i+3)} + n_{\pi(i+4)} + \dots + n_{\pi(N)})].$$

Example 5.3. When j = i + 3, we have

$$\frac{D(\pi') - D(\pi)}{n_{\pi(i)} - n_{\pi(i+3)}} = 3n_{\pi(1)} + 3n_{\pi(2)} + \dots + 3n_{\pi(i-1)} + n_{\pi(i+1)} - n_{\pi(i+2)} - 3n_{\pi(i+4)} - 3n_{\pi(i+5)} - \dots - 3n_{\pi(N)} = 3[(n_{\pi(1)} + n_{\pi(2)} + \dots + n_{\pi(i-1)}) - (n_{\pi(i+4)} + n_{\pi(i+5)} + \dots + n_{\pi(N)})] + (n_{\pi(i+1)} - n_{\pi(i+2)}).$$

From Examples 5.1–5.3, we can see that one can properly assign the values n_1, n_2, \ldots, n_N to attain $D(\pi') < D(\pi)$ sometimes, or $D(\pi') > D(\pi)$ on other occasions. This again shows that the most important aspect for the ordering to attain the optimal maximum is heavily dependent on how large the value is itself of each of the n_1, n_2, \ldots, n_N , and is not purely dependent on the value-ordering of them. In other words, different values of $n_1 \leq n_2 \leq \cdots \leq n_N$ give different orderings for attaining the optimal maximum.

To conclude the paper we propose the following problem.

Problem 5.1. Find a polynomial-time algorithm to compute the ordering for the optimal maximum of D, given $n_1 \leq n_2 \leq \cdots \leq n_N$.

Appendix A. We follow the algorithm of Conjecture 2 for the numerals n_i in Table 1.

 $\begin{aligned} \pi_{max}(R_p) &= \pi_{max}(7) = 6; \\ R_p = 7 - 1 = 6, R = 19 + n_6 = 19 + 18 = 37 \end{aligned}$ Step 4. i = 5; R = 37 > 28 = L, $\pi_{max}(L_p) = \pi_{max}(2) = 5;$ $L_p = 2 + 1 = 3, L = 28 + n_5 = 28 + 17 = 45$ Step 5. i = 4; R = 37 < 45 = L, $\pi_{max}(R_p) = \pi_{max}(6) = 4;$ $R_p = 6 - 1 = 5, R = 37 + n_4 = 37 + 13 = 50$ Step 6. i = 3; R = 50 > 45 = L, $\pi_{max}(L_p) = \pi_{max}(3) = 3;$ $L_p = 3 + 1 = 4, L = 45 + n_3 = 45 + 8 = 53$ Step 7. i = 2; R = 50 < 53 = L, $\pi_{max}(R_p) = \pi_{max}(5) = 2;$ $R_p = 5 - 1 = 4, R = 50 + n_2 = 50 + 5 = 55$ Step 8. i = 1; R = 55 > 53 = L, $\pi_{max}(L_p) = \pi_{max}(4) = 1;$ $L_p = 4 + 1 = 5, L = 53 + n_1 = 53 + 2 = 55$

Finally, we get an ordering π_{max} or $\pi_a = 8, 5, 3, 1, 2, 4, 6, 7$.

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