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A Note on the Inverse Problem for the Wiener Index

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Abstract

It was shown recently that all but 49 positive integers are Wiener index of some tree, which had been conjectured by Lepović and Gutman. In this note we settle the analogous question for unicyclic graphs and also prove that every positive integer which is the Wiener index of some graph (every positive integer other than 2 and 5) is Wiener index of a graph whose cyclomatic number is at most 6. Additional degree restrictions are considered as well.

1 Introduction and statement of results

While most of the literature on graph invariants in mathematical chemistry deals with upper and lower bounds, another interesting type of problem is what is known as the *inverse problem* (see for instance the article [6], in which the inverse problem is discussed

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for various indices): given a certain graph parameter and a value, find a graph (if possible) from a prescribed class that attains this parameter value. This can be stated in a slightly different way as: what parameter values can be attained by graphs in the prescribed class?

One particular instance of an inverse problem concerns the *Wiener index* [10], which was also the first graph invariant to be studied in mathematical chemistry. It is defined as the sum of all distances between pairs of vertices in a graph, i.e.,

$$W(G) = \sum_{\{v,w\} \subseteq V(G)} d(v,w).$$

Many different aspects of the Wiener index have been studied, and multiple variants exist today. Let us refer to [2] and the references therein. If one considers the family of all graphs, then it turns out that almost all positive integers can be obtained as values of the Wiener index, as proven by Gutman, Yeh and Chen [4]:

Theorem 1 *Every positive integer, except for* 2 *and* 5*, is the Wiener index of some connected graph.*

The fact that 2 and 5 cannot be written as Wiener index of a connected graph follows by simple case checking (since any graph on at least four vertices must already have Wiener index ≥ 6). Conversely, a possible way to construct graphs that cover all other values is given by the following simple lemma that we will also need for other purposes:

Lemma 1 *The minimum Wiener index of a connected graph with n vertices and $m \geq n-1$ edges is $n(n-1) - m$.*

This follows obviously from the fact that there are m pairs of vertices whose distance is 1, while all other $\binom{n}{2} - m$ pairs have distance at least 2. Equality holds for any graph that is obtained by adding $m - (n-1)$ edges to a star on n vertices. This lemma also shows that every integer in the interval $[\frac{n(n-1)}{2}, (n-1)^2]$ is Wiener index of some graph; taking the union of these intervals for all $n \geq 2$, one obtains Theorem 1.

A result analogous to Theorem 1 was also obtained for bipartite graphs by Gutman and Yeh [3]. For trees, the situation is slightly more complicated; an exhaustive computer search led Lepović and Gutman [5] to the following conjecture, which was subsequently verified for all integers up to 10^8 [1] and proven independently by Wang and Yu [9] and the author of the present paper [7]:

Theorem 2 *Every positive integer, except for the* 49 *numbers* 2, 3, 5, 6, 7, 8, 11, 12, 13, 14, 15, 17, 19, 21, 22, 23, 24, 26, 27, 30, 33, 34, 37, 38, 39, 41, 43, 45, 47, 51, 53, 55, 60, 61, 69, 73, 77, 78, 83, 85, 87, 89, 91, 99, 101, 106, 113, 147 *and* 159, *is Wiener index of some tree.*

This result was further strengthened in [8], where it was shown that trees with maximum degree ≤ 3 (and therefore, *a fortiori*, chemical trees) are sufficient to cover all but finitely many values. The aim of the present short note is to prove an analogous result for unicyclic graphs and to treat the following question:

Problem 1 Determine the smallest integer k such that every integer that is Wiener index of some connected graph (i.e., any positive integer other than 2 or 5) is Wiener index of a graph whose cyclomatic number is at most k.

It will turn out that the smallest such value is $k = 6$, see Theorem 4 below. For unicyclic graphs, we obtain the following result, which will constitute the main part of this paper:

Theorem 3 *Every positive integer, except for the* 27 *numbers* 1, 2, 4, 5, 6, 7, 9, 10, 11, 12, 13, 14, 18, 19, 20, 21, 22, 23, 25, 30, 32, 33, 34, 36, 37, 49 *and* 50, *is Wiener index of some unicyclic graph.*

If one combines this with Theorem 2, one finds all numbers that are neither Wiener index of a tree nor of a unicyclic graph: 2, 5, 6, 7, 11, 12, 13, 14, 19, 21, 22, 23, 30, 33, 34, 37. While 37 is the Wiener index of the bicyclic graph shown in Figure 1, all other numbers in this list (except for 2 and 5, of course) are covered by Lemma 1 with some $m \leq n + 5$ (equivalently, cyclomatic number ≤ 6) and $n \leq 7$. On the other hand, this is best possible: one can check directly that the maximum Wiener index of a bicyclic graph on ≤ 6 vertices is 28, and clearly this upper bound has to hold for graphs with a larger cyclomatic number as well. On the other hand, Lemma 1 shows that a graph on $n \geq 7$ vertices whose cyclomatic number is at most 5 has Wiener index ≥ 31.

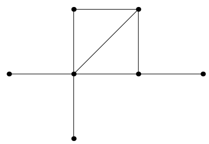

Figure 1: A bicyclic graph whose Wiener index is 37.

Putting everything together, we arrive at the following theorem:

Theorem 4 *Every positive integer other than* 2 *and* 5 *is the Wiener index of some graph of cyclomatic number at most* 6*, and this is best possible in the sense that* 30 *cannot be obtained as Wiener index of any graph whose cyclomatic number is less than* 6*.*

2 Proof of the main result

In order to prove Theorem 3, we slightly adapt the ideas used in [8] for trees to the situation of unicyclic graphs. In fact, we will even prove more: all values that cannot be attained by the Wiener index of a unicyclic graph resp. unicyclic graph with maximum degree ≤ 3 resp. unicyclic graph with maximum degree ≤ 4 (a *chemical* unicyclic graph) will be determined.

To this end, we consider a special family of unicyclic graphs (see Figure 2): it comprises of a 3-cycle, to which paths of length ℓ and m are attached. Furthermore, $k \leq m$ pendant vertices are attached to some of the vertices of the latter path; their positions are denoted by $x_1, x_2, \dots, x_k$ $(1 \leq x_1 < x_2 < \cdots < x_k \leq m)$.

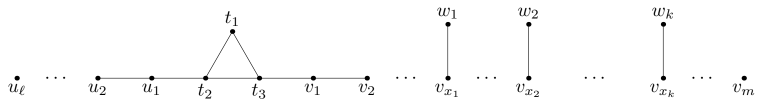

Figure 2: A special family of unicyclic graphs.

The Wiener index of such a unicyclic graph $U(\ell, m, x_1, x_2, \dots, x_k)$ is easily determined as follows:

- The vertices of the path of order $\ell + m + 2$ that is formed by the two attached paths and the vertices t_2, t_3 contributes

$$W(P_{\ell+m+2}) = \binom{\ell+m+3}{3}$$

to the Wiener index.

- The vertex of the triangle that does not lie on this path (t_1 in Figure 2) hat a total distance of
$$\sum_{i=1}^{\ell+1} i + \sum_{j=1}^{m+1} j = \binom{\ell+2}{2} + \binom{m+2}{2}$$
from the vertices on the path.

- The pendant vertex w_k in position x_r has total distance
$$\sum_{i=1}^{x_r+\ell+2} i + \sum_{j=2}^{m-x_r+1} j + (x_r+2) = \binom{x_r+\ell+3}{2} + \binom{m-x_r+2}{2} + x_r + 1$$
from the vertices treated in the first two parts.

- Finally, the total distance between all k pendant vertices $x_1, x_2, \ldots, x_k$ is
$$\sum_{i=1}^{k} \sum_{j=i+1}^{k} (x_j - x_i + 2) = k(k-1) + \sum_{i=1}^{k} (2i-k-1)x_i \ .$$

Hence we obtain the following formula for the Wiener index of $U(\ell, m, x_1, x_2, \ldots, x_k)$:
$$\begin{aligned} W(U(\ell,m,x_1,x_2,\ldots,x_k)) &= \binom{\ell+m+3}{3} + \binom{\ell+2}{2} + \binom{m+2}{2} + k^2 \\ &+ \sum_{i=1}^{k} \left(\binom{x_r+\ell+3}{2} + \binom{m-x_r+2}{2} + (2i-k-1)x_i \right) \end{aligned}$$
Some algebraic manipulations show that this equals
$$\begin{aligned} W(U(\ell,m,x_1,x_2,\ldots,x_k)) &= \binom{\ell+m+3}{3} + \binom{\ell+2}{2} + \binom{m+2}{2} \\ &- \frac{k^3-12k^2-37k}{12} + \frac{k}{4}\left((\ell+m)^2 + 6\ell + 10m\right) \\ &+ \sum_{i=1}^{k} \left(x_i + i + \frac{\ell-m-k+1}{2} \right)^2 . \end{aligned}$$
Now we use the special case $k = 8$ and set $\ell + m = 2s - 1$ for some $s \geq 1$ to obtain
$$\frac{4s^3}{3} + 12s^2 + \left(\frac{101}{3} - 2\ell\right) s + \ell^2 - 7\ell + 29 + \sum_{i=1}^{k} y_i^2,$$
where $y_i = x_i + i + \ell - s - 3$. The integers y_i are restricted by the inequality
$$\ell - s - 1 \leq y_1 < y_2 < \cdots < y_8 \leq s + 4$$

and the additional restriction that no two of them may be consecutive (since $y_{i+1} = x_{i+1} + i + \ell - s - 2 > x_i + i + \ell - s - 2 = y_i + 1$). Next we need the following lemma that was proved in [8, p.1548]:

Lemma 2 *For any* $t \geq 10$*, any integer in the interval* $[224, 5t^2 - 16t + 21]$ *can be represented as the sum of the squares of eight numbers in the interval* $[-t, t]$*, no two of which are consecutive.*

Applying this lemma with $t = s + 1 - \ell$, we find that every integer in the interval

$$I(s,\ell) = \left[\frac{4s^3}{3} + 12s^2 + \left(\frac{101}{3} - 2\ell\right) s + \ell^2 - 7\ell + 253, \right.$$
$$\left. \frac{4s^3}{3} + 17s^2 + \left(\frac{83}{3} - 12\ell\right) s + 6\ell^2 - \ell + 39\right]$$

is the Wiener index of a graph of the form $U(\ell, 2s-1-\ell, x_1, x_2, \ldots, x_8)$ if $s \geq \ell + 9$. We note that both the left and the right endpoint of the interval $I(s,\ell)$ are decreasing as functions of ℓ. Furthermore, consecutive intervals $I(s,\ell-1)$ and $I(s,\ell)$ overlap: this statement is equivalent to the inequality

$$\tfrac{4s^3}{3} + 17s^2 + \left(\tfrac{83}{3} - 12\ell\right) s + 6\ell^2 - \ell + 39 \geq \tfrac{4s^3}{3} + 12s^2 + \left(\tfrac{101}{3} - 2(\ell-1)\right) s + (\ell-1)^2 - 7(\ell-1) + 253,$$

which is in turn equivalent to $5(s-\ell)^2 - 8(s-\ell) \geq 222$, and this is satisfied in view of the condition $s - \ell \geq 9$. Taking the union over all $0 \leq \ell \leq s - 9$, we find that all integers in the interval

$$\left[\tfrac{4s^3}{3} + 11s^2 + \tfrac{80s}{3} + 397, \tfrac{4s^3}{3} + 17s^2 + \tfrac{83s}{3} + 39\right]$$

can be written as the Wiener index of a graph of the form $U(\ell, 2s-1-\ell, x_1, x_2, \ldots, x_8)$. Consecutive intervals of this form overlap for $s \geq 22$, and so we obtain the following proposition:

Proposition 3 *Every integer* ≥ 20505 *is the Wiener index of a unicyclic graph of the form* $U(\ell, m, x_1, x_2, \ldots, x_8)$*.*

The remaining set of integers is treated by means of a computer search. All files can be found at `http://math.sun.ac.za/~swagner/InverseWiener`. The first part of this computer search, which already reduces the problem greatly, is to consider graphs of the form $U(\ell, m, x_1, x_2, \ldots, x_k)$ for arbitrary k. It is sufficient to consider $\ell, m \leq 25$ and $k \leq 10$ to obtain the following result:

Proposition 4 *Every integer* ≥ 523 *is the Wiener index of a unicyclic graph of the form* $U(\ell, m, x_1, x_2, \ldots, x_k)$.

In a next step, consider all unicyclic graphs of girth 3 with at up to 24 vertices whose maximum degree is 3 to obtain

Proposition 5 *Every integer* ≥ 190 *is the Wiener index of a unicyclic graph whose girth and maximum degree are* 3.

These calculations can be carried out quite effectively as follows: note that every such unicyclic graph comprises of three trees, rooted at the vertices of the unique cycle, with the property that the root has degree 1 (or 0) and all other vertices have degree at most 3. Instead of generating all trees of this form, we only determine all possible triples (n, d, w), where n is the order, d the sum of all distances to the root, and w the Wiener index of a tree of this form. This can be done by a simple recursion. It is sufficient to know such triples only: if (n_1, d_1, w_1), (n_2, d_2, w_2), (n_3, d_3, w_3) are the triples associated to the three trees, then the Wiener index of the corresponding unicyclic graph is found to be

$$w_1 + w_2 + w_3 + d_1(n_2 + n_3) + d_2(n_1 + n_3) + d_3(n_1 + n_2) + n_1 n_2 + n_1 n_3 + n_2 n_3 \ .$$

Making use of this formula, it is now easy to determine all possible Wiener indices of unicyclic graphs of order ≤ 24 with girth and maximum degree 3.

For the remaining interval, a brute-force search can be carried out: considering unicyclic graphs with maximum degree ≤ 3 and order ≤ 12, we obtain the following result:

Theorem 5 *Every positive integer other than* 1, 2, 4, 5, 6, 7, 9, 10, 11, 12, 13, 14, 18, 19, 20, 21, 22, 23, 24, 25, 30, 32, 33, 34, 35, 36, 37, 38, 39, 49, 50, 52, 53, 54, 55, 56, 57, 65, 75, 76, 77, 79, 81 *and* 106 *is the Wiener index of a unicyclic graph with maximum degree* ≤ 3.

It is not necessary to consider unicyclic graphs of order greater than 12 since the smallest possible Wiener index of a unicyclic graph of order ≥ 13 is already 143 by Lemma 1. Likewise, we can determine the Wiener index of all unicyclic graphs of order ≤ 10 whose maximum degree is 4 to reduce this list as follows:

Theorem 6 *Every positive integer other than* 1, 2, 4, 5, 6, 7, 9, 10, 11, 12, 13, 14, 18, 19, 20, 21, 22, 23, 24, 25, 30, 32, 33, 34, 35, 36, 37, 38, 49, 50, 52, 53, 54, 55 *and* 76 *is the Wiener index of a unicyclic graph with maximum degree* ≤ 4.

Finally, we remove the condition on the degrees and consider all unicyclic trees of order ≤ 9 (which is sufficient by the aforementioned argument) to prove Theorem 3.

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