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ORIGINAL PAPER

Terminal Wiener index

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Abstract Motivated by some recent research on the terminal (reduced) distance matrix, we consider the *terminal Wiener index* (TW) of trees, equal to the sum of distances between all pairs of pendent vertices. A simple formula for computing TW is obtained and the trees with minimum and maximum TW are characterized.

Keywords Wiener index · Terminal Wiener index · Distance (in graph) · Tree · Terminal vertex · Pendent vertex

1 Introduction

Let G be a connected graph on n vertices, whose vertices are labelled by $v_1, v_2, \ldots, v_n$. The distance $d(v_i, v_j|G)$ between two vertices v_i and v_j of G is equal to the length (= number of edges) of the shortest path that connects v_i and v_j [1]. The square matrix of order n whose (i, j)-entry is $d(v_i, v_j|G)$ is called the distance matrix of G.

In a number of recent studies, the so-called *terminal distance matrix* [2,3] or *reduced distance matrix* [4] of trees was considered. If an n-vertex tree T has k pendent vertices (= vertices of degree one), labelled by $v_1, v_2, \ldots, v_k$, then its terminal distance matrix is the square matrix of order k whose (i, j)-entry is $d(v_i, v_j|T)$. Recall that for any n-vertex tree, $2 \leq k \leq n - 1$. The (unique) n-vertex trees with $k = 2$ and $k = n - 1$ are, respectively, the *path* (P_n) and the *star* (S_n).

Terminal distance matrices were used in the mathematical modelling of proteins and genetic codes [2,3,5], and were proposed to serve as a source of a whole class of molecular-structure descriptors [3,4]. It is worth noting that the terminal distance

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matrix of a tree T determines the entire distance matrix of T, and thus fully determines the tree T itself [6]. It is easy to envisage that in the terminal distance matrix of a non-tree graph G, the information on the structure of G can be almost completely missing: just think of an arbitrary graph possessing exactly two pendent vertices, both adjacent to the same vertex.

One of the oldest and most thoroughly studied molecular-structure descriptors is the Wiener index [7], the sum of the distances between all pairs of vertices of a given graph G:

$$W(G) = \sum_{1 \le i < j \le n} d(v_j, v_j | G).$$

For details on the Wiener index see the reviews [8,9], the recent papers [10–17] and the references cited therein.

Motivated by the previous researches on the terminal distance matrix and on its chemical applications [2–6] we now define the *terminal Wiener index* $TW(T)$ of a tree T as *the sum of the distances between all pairs of pendent vertices*. More formally,

$$TW(T) = \sum_{1 \le i < j \le k} d(v_j, v_j | T). \tag{1}$$

As before, in Eq. 1 it is assumed that the tree T has n vertices of which k vertices, labelled by $v_1, v_2, \ldots, v_k$, are pendent.

In order to illustrate the above definition, we show how the terminal Wiener index is computed for the tree T_1 depicted in Fig. 1. Here we directly apply Eq. 1.

The tree T_1 has six pendent vertices—$v_1, v_2, \ldots, v_6$. Therefore the summation on the right-hand side of (1) contains $\binom{6}{2} = 15$ terms, and we have:

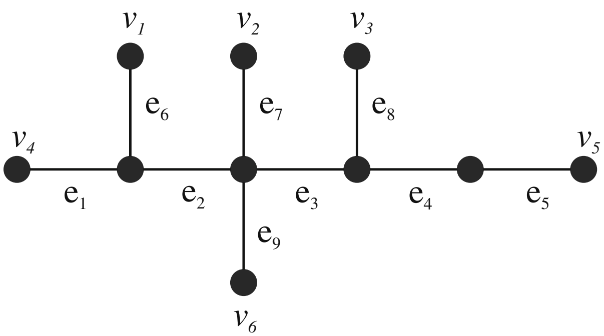

Fig. 1 A tree whose terminal Wiener index is equal to 51

$$\begin{aligned} TW(T_1) &= d(v_1, v_2|T_1) + d(v_1, v_3|T_1) + d(v_1, v_4|T_1) + d(v_1, v_5|T_1) + d(v_1, v_6|T_1) \\ &\quad + d(v_2, v_3|T_1) + d(v_2, v_4|T_1) + d(v_2, v_5|T_1) + d(v_2, v_6|T_1) + d(v_3, v_4|T_1) \\ &\quad + d(v_3, v_5|T_1) + d(v_3, v_6|T_1) + d(v_4, v_5|T_1) + d(v_4, v_6|T_1) + d(v_5, v_6|T_1) \\ &= 3 + 4 + 2 + 5 + 3 + 3 + 3 + 4 + 2 + 4 + 3 + 3 + 5 + 3 + 4 = 51. \end{aligned}$$

2 A modified Wiener's "first theorem"

The first question that should be asked in connection with the terminal Wiener index is how it could be efficiently computed. For this we offer a result that is fully analogous to Wiener's "first theorem" for the ordinary Wiener index [7,8].

In his seminal article [7] Wiener communicated the formula

$$W(T) = \sum_{e} n_1(e) \cdot n_2(e) \tag{2}$$

which holds for any tree T. This result may be viewed as the first theorem ever for the Wiener index. In formula (2) e stands for an edge, whereas $n_1(e)$ and $n_2(e)$ are the number of vertices lying on the two sides of e; the summation in (2) goes over all edges of the respective tree T. If T has n vertices, then $n_1(e) + n_2(e) = n$ for all edges e.

In the paper [7] no proof of formula (2) was put forward. The proof of (2) is easy [18]: Instead of summing the distances (= the number of edges in the shortest paths) between all pairs of vertices in the tree T, we may count how many times a particular edge e lies on the (unique) shortest path between two vertices, and then add these counts over all edges of the underlying tree. The number of shortest paths that go through the edge e is equal to $n_1(e) \cdot n_2(e)$.

Using the same idea we obtain:

Theorem 1 *Let T be an n-vertex tree with k pendent vertices, and let e be its edge. Denote by $p_1(e)$ and $p_2(e)$ the number of pendent vertices of T, lying on the two sides of e. Then*

$$TW(T) = \sum_{e} p_1(e) \cdot p_2(e) \tag{3}$$

with the summation embracing all the $n - 1$ edges of T.

Proof Instead of summing the distances between all pairs of pendent vertices in the tree T, we count how many times a particular edge e lies on the shortest path between two pendent vertices, and then add these counts over all edges of the underlying tree. Such shortest paths will start at $p_1(e)$ pendent vertices (those lying on one side of e) and end at $p_2(e)$ pendent vertices (those lying on the other side of e). Thus their number is $p_1(e) \cdot p_2(e)$, which leads to Eq. 3. □

In should be noted that for all edges of the tree T,

$$p_1(e) + p_2(e) = k \quad \text{and} \quad p_1(e), p_2(e) \geq 1.$$

Consequently,

$$k - 1 \leq p_1(e) \cdot p_2(e) \leq \left\lfloor \frac{k}{2} \right\rfloor \left\lceil \frac{k}{2} \right\rceil.$$

If e is a pendent edge, then $p_1(e) \cdot p_2(e) = k - 1$.

For the tree T_1 (see Fig. 1) we immediately get:

$$\begin{array}{ll}
p_1(e_1) = 1;\ p_2(e_1) = 5 & p_1(e_2) = 2;\ p_2(e_2) = 4 \\
p_1(e_3) = 4;\ p_2(e_3) = 2 & p_1(e_4) = 5;\ p_2(e_4) = 1 \\
p_1(e_5) = 5;\ p_2(e_5) = 1 & p_1(e_6) = 1;\ p_2(e_6) = 5 \\
p_1(e_7) = 1;\ p_2(e_7) = 5 & p_1(e_8) = 1;\ p_2(e_8) = 5 \\
p_1(e_9) = 1;\ p_2(e_9) = 5 &
\end{array}$$

and therefore formula (3) yields:

$$\begin{aligned} TW(T_1) = {} & (1 \times 5) + (2 \times 4) + (4 \times 2) + (5 \times 1) + (1 \times 5) \\ & + (1 \times 5) + (1 \times 5) + (1 \times 5) + (1 \times 5) = 51. \end{aligned}$$

This example shows that the calculation of TW by means of formula (3) is somewhat easier than by using the Definition 1. However, the true value of formula (3) is in enabling one to deduce a number of general properties of the terminal Wiener index.

3 The tree with minimal terminal Wiener index

For the considerations that follow one should recall that the summation on the right-hand side of (3) goes over $n - 1$ (non-zero) terms.

As further simple examples of the application of formula (3) we compute the terminal Wiener index of the star and the path.

In the case of the star S_n, there are $n - 1$ pendent vertices, and all edges are pendent. Therefore for all edges of the star, $p_1(e) = 1,\ p_2(e) = n - 2$, resulting in $TW(S_n) = (n - 1)[1 \times (n - 2)] = (n - 1)(n - 2)$.

In the case of the path P_n, there are two pendent vertices, and for all edges $p_1(e) = p_2(e) = 1$. Therefore, $TW(P_n) = (n - 1)[1 \times 1] = n - 1$.

Because 1 is the minimal possible value for the product $p_1(e) \cdot p_2(e)$, it immediately follows that $n - 1$ is the minimal possible value that the terminal Wiener index may assume for n-vertex trees. Because any tree different from P_n possesses at least one edge e for which $p_1(e) \cdot p_2(e) \geq 2$, we conclude that $TW(T) > n - 1$ holds for all n-vertex trees $T \ncong P_n$. By this, as a straightforward consequence of Eq. 3 we obtained:

Theorem 2 *For any n-vertex tree,* $TW(T) \geq n - 1$. *Equality* $TW(T) = n - 1$ *holds if and only if* $T \cong P_n$. □

Thus the path is the tree with minimal terminal Wiener index. The finding of the tree(s) with maximal TW is less easy and will be achieved in the subsequent sections.

4 Trees with fixed number of pendent vertices having minimal and maximal terminal Wiener index

In this section we restrict our consideration to n-vertex trees having a fixed number k of pendent vertices. Such trees have also k pendent edges, and, consequently, k summands on the right-hand side of Eq. 3 are equal to $k-1$. Formula (3) can thus be rewritten as

$$TW(T) = k(k-1) + \sum_{e'} p_1(e') \cdot p_2(e') \tag{4}$$

where e' are the non-pendent edges of T. Note that there exist $n-1-k$ such edges.

The only n-vertex tree with $k = 2$ is the path P_n. Therefore, in what follows, we assume that $3 \leq k \leq n-1$.

In view of the fact that $p_1(e') + p_2(e') = k$, the minimal value of the product $p_1(e') \cdot p_2(e')$ is $k-1$. Therefore, if for all non-pendent edges e' the product $p_1(e') \cdot p_2(e')$ is equal to $k-1$, then the respective tree will have minimal possible TW-value. Such trees do exist.

A tree is said to be *starlike of degree k* if exactly one of its vertices has degree greater than two, and this degree is equal to k, $k \geq 3$. In Fig. 2 are depicted all 12-vertex starlike trees of degree 4.

Theorem 3 *Among n-vertex trees with a fixed number k of pendent vertices, $k \geq 3$, the starlike trees of degree k have minimal terminal Wiener index. All n-vertex starlike trees of degree k have $TW = (n-1)(k-1)$.*

Proof It is easy to see that among trees, only the starlike trees have the property that either $p_1(e) = 1$ or $p_2(e) = 1$ holds for any edge e. □

From Theorem 3 we see that $TW = 33$ holds for all the eleven trees depicted in Fig. 2. From this example one concludes that there are numerous non-isomorphic trees having the same TW-value. In other words, the isomer-discriminating power of the terminal Wiener index is very low. In particular, all trees with 3 pendent vertices are starlike, and thus all such trees with same number n of vertices have same TW-values, equal to $2(n-1)$.

We now begin the search for trees with k pendent vertices and maximal TW. For reason just explained, we are not interested in the case $k = 3$.

Bearing in mind that the maximal possible value of the product $p_1(e') \cdot p_2(e')$ is $\lfloor k/2 \rfloor \cdot \lceil k/2 \rceil$, from Eq. 4 we conclude that the maximal possible value of TW is $k(k-1) + (n-1-k)\lfloor k/2 \rfloor \lceil k/2 \rceil$, provided that there exist n-vertex trees with k pendent vertices, for which all non-pendent edges e' have the property

$$p_1(e') \cdot p_2(e') = \left\lfloor \frac{k}{2} \right\rfloor \left\lceil \frac{k}{2} \right\rceil . \tag{5}$$

Indeed, such trees do exist (see below). We thus arrive at:

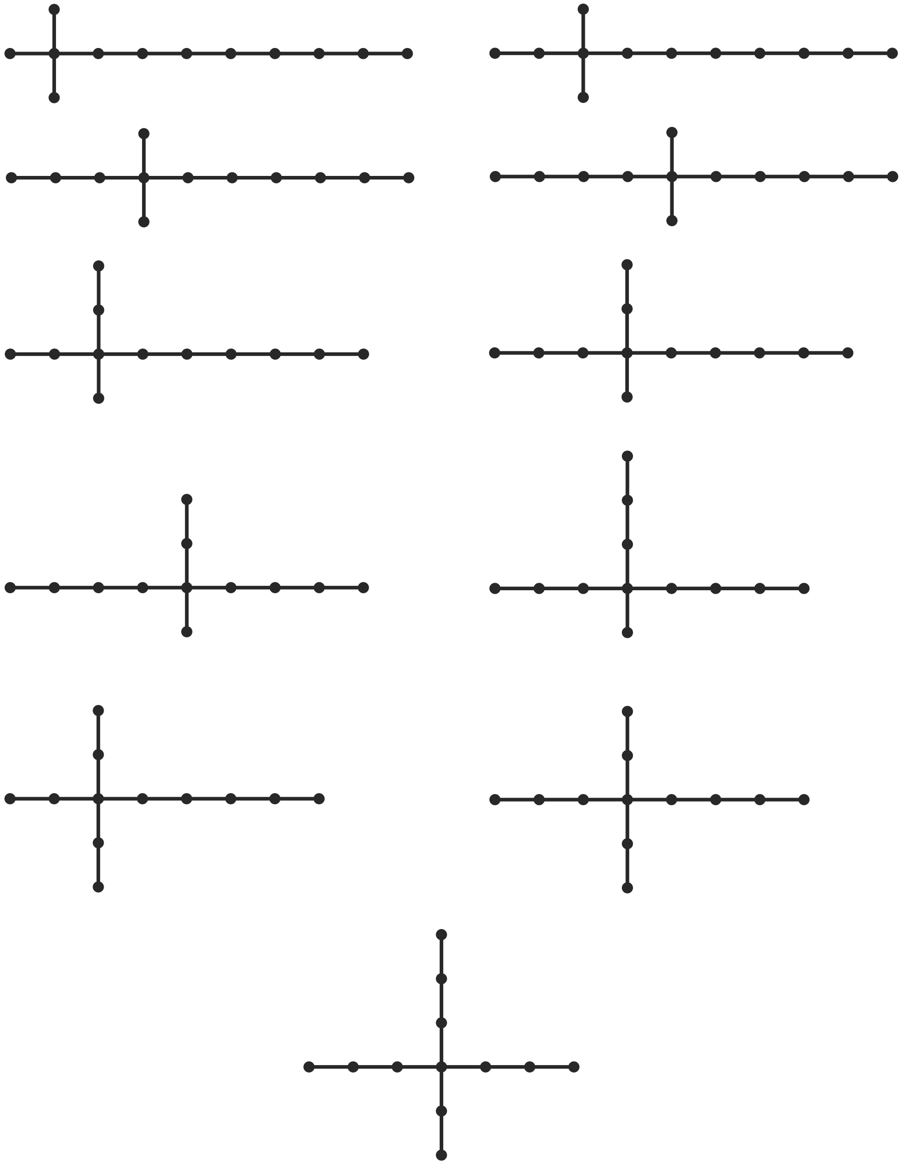

Fig. 2 The 12-vertex starlike trees of degree 4. Among 12-vertex trees with 4 pendent vertices these all have minimal terminal Wiener index, equal to 33

Theorem 4 *Among n-vertex trees with a fixed number k of pendent vertices, $k \geq 4$, the trees whose all non-terminal edges e' satisfy condition (5) have maximal terminal Wiener index. All such trees have*

$$TW = k(k-1) + (n-1-k)\left\lfloor \frac{k}{2} \right\rfloor \left\lceil \frac{k}{2} \right\rceil . \tag{6}$$

Proof We have already seen that the right-hand side of Eq. 6 is the maximal possible value that TW may assume. What remains is to demonstrate that there are trees satisfying Eq. 6. The construction of such trees proceeds as follows:

(a) If k is even, $4 \leq k < n-1$, then the required tree is obtained from the path P_{n-k} by attaching to each of its terminal vertices $k/2$ new pendent vertices. This tree is unique.

(b) If k is odd, $5 \leq k < n-1$, then the required tree is obtained from the path P_{n-k} by attaching to each of its terminal vertices $(k-1)/2$ new pendent vertices, and by attaching one more pendent vertex to some vertex of P_{n-k}. There exist $\lceil (n-k)/2 \rceil$ distinct trees of this kind.

(c) If $k = n-1$, then the respective tree is the star, having no non-pendent edges at all.

It can easily be verified that the above described trees have n vertices, k pendent vertices and that their non-pendent edges satisfy condition (5). It is also straightforward to see that these are the only trees with such properties. □

The trees with 12 vertices and various number of pendent vertices, having maximal terminal Wiener index are shown in Fig. 3.

5 Trees with maximal terminal Wiener index

In the preceding section we determined the n-vertex trees with a fixed number k of pendent vertices, for which TW is maximal. In order to find the n-vertex tree(s) for which TW is maximal we only have to determine the value of k for which the right-hand side of Eq. 6 is maximal. This is an elementary, yet not easy mathematical task. By solving it we obtain:

Theorem 5 *Within the class of all trees with n vertices the following holds.*

(a) If $3 \leq n \leq 9$, then the star S_n has maximal terminal Wiener index, equal to $(n-1)(n-2)$.

(b) If $n = 3s,\ s = 4, 5, 6, \ldots$, then the tree with $k = 2s+2$ pendent vertices (specified in the proof of Theorem 4) has maximal terminal Wiener index, equal to $s^3 + 3s^2 + s - 1$. This tree is unique.

(c) If $n = 3s+1,\ s = 3, 4, 5, \ldots$, then the trees with $k = 2s+2$ and $k = 2s+3$ pendent vertices (specified in the proof of Theorem 4) have maximal terminal Wiener indices, all equal to $s^3 + 4s^2 + 3s$. There are $\lceil s/2 \rceil$ distinct trees of this kind.

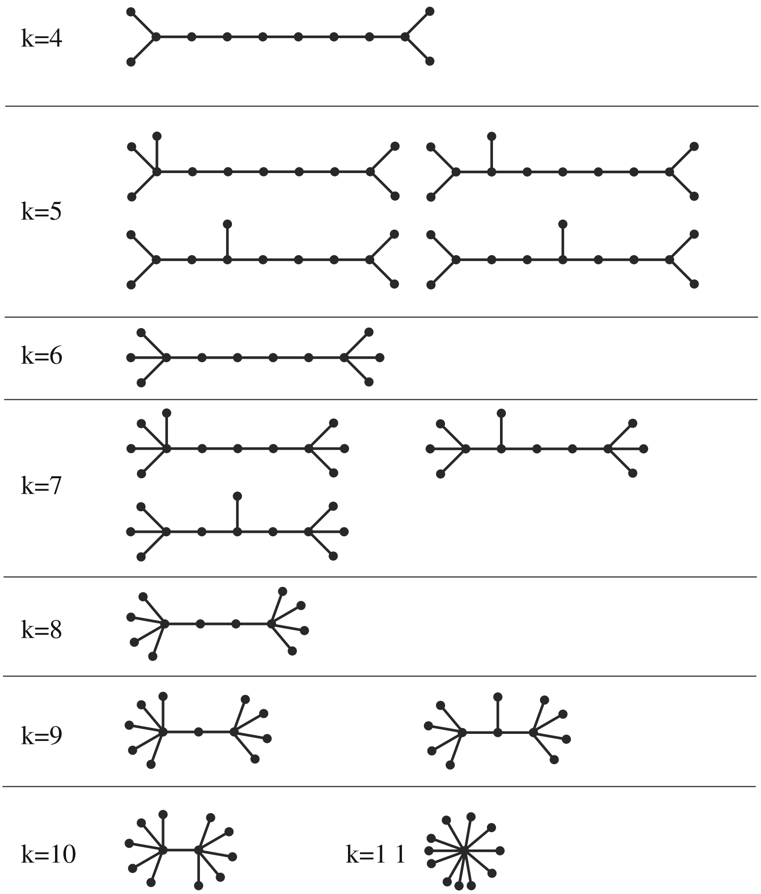

Fig. 3 Trees with $n = 12$ vertices and k pendent vertices, having maximal terminal Wiener index. For even values of k such trees are unique. For odd values of k there exist $\lceil (n-k)/2 \rceil$ distinct trees of this kind; in particular, 4, 3, 2, and 1 for $k = 5$, $k = 7$, $k = 9$, and $k = 11$, respectively

(d) *If* $n = 3s + 2,\ s = 3, 4, 5, \ldots,$ *then the trees with* $k = 2s + 3$ *pendent vertices (specified in the proof of Theorem 4) have maximal terminal Wiener indices, all equal to* $s^3 + 5\,s^2 + 6s + 2$. *There are* $\lceil (s-1)/2 \rceil$ *distinct trees of this kind.*

In Fig. 4 *are depicted all n-vertex trees with maximal terminal Wiener index, for* $9 \leq n \leq 16$.

Proof of Theorem 5 will be only sketched. First, the solutions for $n \leq 9$ have to be found by direct checking, which is easy. Then, bearing in mind Eq. 6, and the fact that

$$\left\lfloor \frac{k}{2} \right\rfloor \left\lceil \frac{k}{2} \right\rceil = \begin{cases} k^2/4 & \text{if } k \text{ is even} \\ (k^2-1)/4 & \text{if } k \text{ is odd} \end{cases}$$

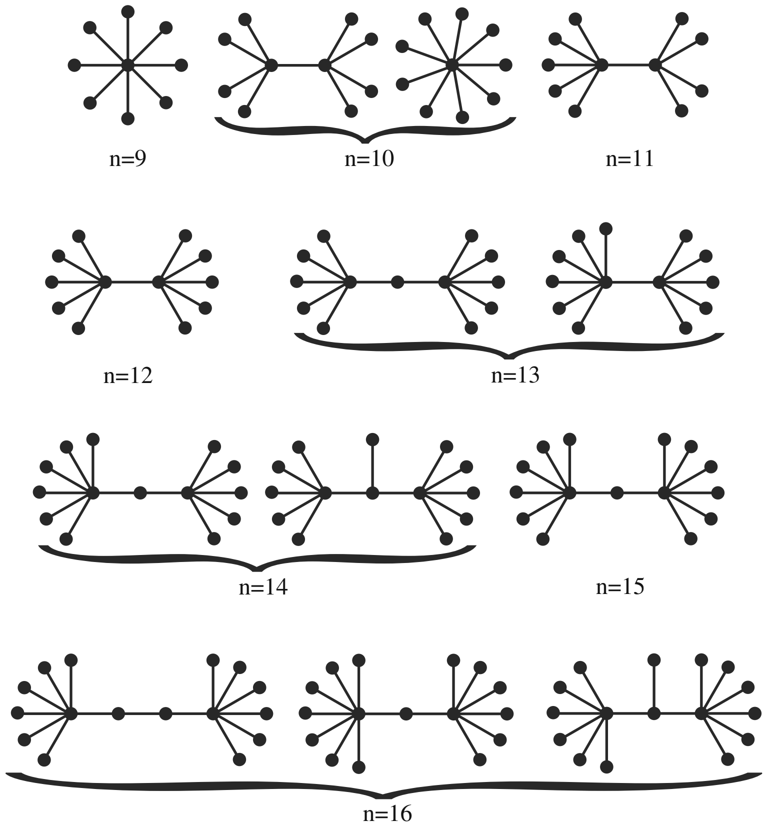

Fig. 4 The n-vertex trees with maximal terminal Wiener index, for $n = 9, 10, \ldots, 16$

we define two auxiliary functions:

$$f_1(x) = x(x-1) + (n-1-x)\,\frac{x^2}{4}$$
$$f_2(k) = x(x-1) + (n-1-x)\,\frac{x^2-1}{4}$$

and find the value of the variable x, say $x_{1,max}$ and $x_{2,max}$, for which these become maximal. Because $x_{1,max}$ is not integer, we round it to the nearest smaller and nearest greater even integer. Analogously, we round $x_{2,max}$ to the nearest smaller and nearest greater odd integer. Next, we set k equal to each of these four values, and compute the right-hand side of Eq. 6. Four cubic polynomials in n are thus obtained, and we choose the one (or those two) which have the greatest value. This procedure has to be done separately for the cases $n \equiv 0\ (mod\ 3)$, $n \equiv 1\ (mod\ 3)$, and $n \equiv 2\ (mod\ 3)$. Theorem 6 follows. □

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