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Research Paper

Multiplicative Zagreb Indices and Extremal Complexity of Line Graphs

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(Dedicated to the memory of Professor Ali Reza Ashrafi.)

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Abstract

The number of spanning trees of a graph G is called the complexity of G. It is known that the complexity of the line graph of a given graph G can be computed as the sum over all spanning trees of G of contributions which depend on various types of products of degrees of vertices of G. We interpret the contributions in terms of three types of multiplicative Zagreb indices, obtaining simple and compact expressions for the complexity of line graphs of graphs with low cyclomatic numbers. As an application, we determine the unicyclic graphs whose line graphs have the smallest and the largest complexity.

1 Introduction

Given two graphs on the same number of vertices, one can often intuitively perceive one of them as more complex that the other. However, the intuitive perception of complexity turns out to be somewhat elusive when it comes to its quantification. Several different measures of graph complexity were proposed, each with its own good and less good sides. The most standard one is the number of spanning trees.

There are several standard ways of counting spanning trees, such as, e.g., the contraction-deletion theorem and the matrix-tree theorem. In most cases, they will not produce simple closed formulas for the number of spanning trees in terms of some simple structural parameters of the considered graph. It is, hence, of interest to consider special cases for which such formulas can be obtained. In this paper, we start from one such result, expressing the number of spanning trees of the line graph $L(G)$ of a graph G in terms of sums and products of degrees of vertices of G. The expressions appearing there are reinterpreted in terms of three well-known topological indices, resulting in compact formulas for the complexity of the line graph of G. When G itself

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has a low cyclomatic number, the obtained formulas allow for determining the graphs whose line graphs achieve the extremal complexities.

In the next section, we give the necessary definitions and quote some preliminary results. Section 3 contains our main results on the complexity of line graphs of unicyclic graphs. In the last section, we summarize our findings and indicate some possible directions for further research.

2 Definitions and preliminary results

All graphs we consider here are simple and connected. We assume that the reader is familiar with those terms, as well as with other basic terms such as, e.g., vertices, edges, degrees, paths and cycles. For any doubts, we refer the reader to some standard monographs on graph theory [1, 2].

For a graph G, we denote its set of vertices by $V(G)$, and its set of edges by $E(G)$. When there is no risk of confusion, we shorten the notation to V and E, respectively. If a graph F contains no cycles, one says that F is an *acyclic* graph. A graph whose every component is acyclic is called a *forest*. A *tree* T is a connected acyclic graph, a forest with exactly one connected component. For a connected graph G with n vertices and m edges, we define its *cyclomatic number* $c(G)$ as $c(G) = m - n + 1$. (The definition can be made meaningful also for graphs with several connected components by replacing 1 with the number of components.) Hence, trees are connected graphs with the cyclomatic number zero. Graphs with $c(G) = 1$ are called *unicyclic graphs*; generally, graphs with $c(G) = k$ are called k-cyclic.

A subgraph H of a graph G is *spanning* if it includes all vertices (but not necessarily all edges) of G. A subgraph H is *induced* if all edges between vertices of H in G appear also in H. A connected acyclic subgraph T of G is a *spanning tree* in G if it includes all vertices of G. The number of spanning trees of a (connected) graph G is called the *complexity* of G and denoted by $\tau(G)$.

For a given graph G, its *line graph* $L(G)$ is defined as the graph whose vertices are edges of G, and two vertices in $L(G)$ are connected by an edge if and only if the corresponding edges in G are incident to the same vertex in G. The line graph of a connected graph is itself connected. It is well known that not every connected graph is a line graph. There are several small graphs which cannot appear as induced subgraphs of line graphs [3].

A *topological index* is a numerical quantity assigned to a graph G which remains invariant under graph isomorphisms. It is, usually, derived from some structural properties of G. The main motivation for the study of topological indices comes from their role in the QSAR/QSPR studies. Many topological indices have been introduced and studied so far. We refer the reader to [4] and references therein for more background. In the chemical context, topological indices are also known as *molecular descriptors*, reflecting their use in the study of physico-chemical properties of various chemical compounds.

The two oldest named topological indices, the Wiener index and the Platt index, were introduced almost simultaneously back in 1947, the Wiener index [5] preceding the other one [6] by mere five months. A long period of dormancy ensued, punctuated by sporadic publications [7, 8]. The activities resumed at the beginning of seventies, by introducing a pair of indices by a group of researchers working at the Rudjer Bošković Institute in Zagreb, Croatia, which subsequently became known as the *Zagreb group indices* and later simply as the *Zagreb indices* [9]. See a nice paper by Gutman [10] for more historical details.

The *first Zagreb index* $M_1(G)$ and the *second Zagreb index* $M_2(G)$ of a graph G are defined, respectively, as the sum over all vertices of G of squares of their degrees, and the sum over all edges of G of products of degrees of their end-vertices:

$$M_1(G) = \sum_{v \in V(G)} d_v^2, \qquad M_2(G) = \sum_{uv \in E(G)} d_u d_v.$$

(Here d_u denotes the degree of the vertex $u \in V$.) The first Zagreb index was also studied in the mathematical literature, by researchers apparently unaware of its chemical relevance [11–13]. It was observed much later [14] that the first Zagreb index has an alternative, bond-additive, formulation, as the sum over all edges of G of sums of degrees of their end-vertices,

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v).$$

As often is the case with topological indices, the Zagreb indices were soon generalized in several ways, giving rise to several derived indices. In this paper, we are concerned with two indices that arise by replacing sums with products in the defining relations of $M_1(G)$ and $M_2(G)$. The resulting invariants, named the *multiplicative Zagreb indices*, were introduced by Todeschini and his coauthors in 2010 [15, 16]. The first and the second multiplicative Zagreb index are defined, respectively, as follows:

$$\Pi_1(G) = \prod_{v \in V(G)} d_v^2, \qquad \Pi_2(G) = \prod_{uv \in E(G)} d_u d_v.$$

An alternative version of the first multiplicative Zagreb index, based on the bond-additive formulation, was proposed by Eliasi, Iranmanesh and Gutman [17],

$$\Pi_1^*(G) = \prod_{uv \in E(G)} (d_u + d_v).$$

This alternative version became known as the *multiplicative sum Zagreb index* [18]. The first multiplicative Zagreb index is closely related to another index, the Narumi–Katayama index, defined as the product of degrees of all vertices of a graph, $NK(G) = \prod_{v \in V(G)} d_v$. It was introduced by Narumi and Katayama in 1984 [19] and modestly named the "simple topological index". We refer the reader to [20] and references therein for more information on the history and uses of the Narumi–Katayama index. As the first multiplicative Zagreb index is nothing else but the square of the Narumi–Katayama index, $\Pi_1(G) = NK(G)^2$, they capture the same information carried by the degree-sequence of a graph, and can be used interchangeably. Notice that, unlike the original Zagreb indices, the two multiplicative versions of the first Zagreb index behave in different ways.

It turns out that it is much easier to introduce a new topological index than to find a good use for it. Certainly, some indices deserve studying because they have interesting and non-trivial properties, but in many cases, the new indices struggle to find some application. One of the goals of this note is to point to a potential application of multiplicative Zagreb indices for computing complexities of line graphs of graphs with low cyclomatic number, in particular of line graphs of trees and unicyclic graphs.

Our starting point is the following result (Theorem 3.1 of [21]):

Theorem 2.1. *Let G be a loopless graph and let $\mathcal{T}(G)$ be the set of all spanning trees of G. Then*

$$\tau(L(G)) = \frac{1}{\prod_{v \in V(G)} d_v^2} \sum_{T \subseteq \mathcal{T}(G)} \left[\prod_{e=xy \in E(T)} d_x d_y \right] \left[\prod_{e=uv \in E(G) \setminus E(T)} [d_u + d_v] \right].$$

The above expression involves the sum running over all spanning trees of G. All three types of products appearing there look familiar, and one could be tempted to interpret the right-hand side as

$$\frac{1}{\Pi_1(G)} \sum_{T \subseteq \mathcal{T}(G)} \Pi_2(T)\Pi_1^*(G - E(T)).$$

It would be incorrect, though, as the degrees of vertices in the last two products are taken in G, not in T. In the next section, we investigate how much of this approach could be salvaged when the number of spanning trees of G is small.
We refer the reader to [22, 23] for more results of the type quoted in Theorem 2.1.

3 Main results

3.1 Trees

The simplest possible situation arises when G itself is a tree. In that case, $G = T$, there is only one term in the sum, the second product is empty, and the degrees of vertices in G and T coincide. Hence, Theorem 2.1 reduces to a very simple expression.

Corollary 3.1. *Let T be a tree and $L(T)$ its line graph. Then* $\tau(L(T)) = \frac{\Pi_2(T)}{\Pi_1(T)}$.

The above result can be further simplified by applying formula

$$\sum_{u \in V(G)} F(u) = \sum_{uv \in E(G)} \left[\frac{F(u)}{d_u} + \frac{F(v)}{d_v}\right],$$

valid for any numerical quantity $F(u)$ depending on the degree d_u [14]. By taking the logarithm of $\Pi_2(G)$ and applying the above formula backwards, we obtain

$$\log \Pi_2(G) = \sum_{uv \in E(G)} [\log d_u + \log d_v] = \sum_{v \in V(G)} d_u \log d_u = \log \prod_{u \in V(G)} {d_u}^{d_u},$$

which, plugged into the right-hand side of Corollary 3.1, yields an alternative formula for the complexity of the line graph of a tree T.

Corollary 3.2. *Let T be a tree and $L(T)$ its line graph. Then*

$$\tau(L(T)) = \prod_{u \in V(G)} {d_u}^{d_u - 2}.$$

The above logarithmic trick also establishes another equivalence between two topological indices: the quantity $\prod_{u \in V(G)} {d_u}^{d_u}$, introduced in this form by Ghorbani *et al.* [24] and since known as the *modified Narumi–Katayama index* $NK^*(G)$, is identical to the second multiplicative Zagreb index.

We close the subsection on trees by noticing that the formula of Corollary 3.2 readily yields both extremal cases for trees. It returns 1 for any path $T = P_n$, since degrees 1 and 2 contribute 1 to the product, and it returns the Cayley formula $\tau(K_n) = n^{n-2}$ for the line graph K_n of the star $T = K_{1,n}$.

3.2 Unicyclic graphs

The next simplest case in Theorem 2.1 is when G is a unicyclic graph. Each unicyclic graph U_n on n vertices contains an induced cycle C_k of length k, where $3 \leq k \leq n$, and some number of trees, $T_1, \ldots, T_l$, rooted at the vertices of C_k. It is sometimes convenient to assume that there are exactly k such trees, allowing for some of them to be empty. The length of the unique cycle of U_n will be called its *girth*.

Proposition 3.3. *Let U_n be a unicyclic graph, $L(U_n)$ its line graph, and let C_k be the unique cycle in U_n, induced by the vertices $v_1, \ldots, v_k$. Then*

$$\tau(L(U_n)) = 2\ \frac{\Pi_2(U_n)}{\Pi_1(U_n)}\ \sum_{i=1}^{k} \frac{1}{d_{v_i}} = 2 \left[\prod_{u \in V(U_n)} d_u^{\,d_u - 2} \right] \sum_{i=1}^{k} \frac{1}{d_{v_i}}.$$

Proof. Let C_k be the unique cycle in U_n induced by the vertices $v_1, \ldots, v_k$. Then U_n has exactly k spanning trees, each obtained by removing exactly one edge $v_i v_{i+1}$, where the indices are counted modulo k. For each such spanning tree, its complement has exactly one edge, so the second product in the right-hand side of Theorem 2.1 has only one term. The first product in each summand includes all edges except one, the one not participating in the corresponding spanning tree. Hence, it evaluates to the whole second multiplicative Zagreb index of U_n divided by $d_{u_i} d_{u_{i+1}}$, the contribution of the missing edge. By taking this into account, we obtain

$$\begin{aligned}
\tau(L(U_n)) &= \frac{1}{\Pi_1(U_n)} \sum_{i=1}^{k} \left[\prod_{\substack{xy \in E(U_n) \\ xy \neq v_i v_{i+1}}} d_x d_y \right] \left(d_{v_i} + d_{v_{i+1}} \right) \\
&= \frac{\Pi_2(U_n)}{\Pi_1(U_n)} \sum_{i=1}^{k} \frac{d_{v_i} + d_{v_{i+1}}}{d_{v_i} d_{v_{i+1}}} \\
&= \left[\prod_{u \in V(U_n)} d_u^{\,d_u - 2} \right] \sum_{i=1}^{k} \left[\frac{1}{d_{v_i}} + \frac{1}{d_{v_{i+1}}} \right] \\
&= 2 \left[\prod_{u \in V(U_n)} d_u^{\,d_u - 2} \right] \sum_{i=1}^{k} \frac{1}{d_{v_i}}.
\end{aligned}$$

∎

For the trivial case $U_n = C_n$, the above theorem clearly gives the correct answer, $\tau(L(C_n)) = \tau(C_n) = n$. By taking a closer look at the formula, one can notice that it will be dominated by the first term, since the sum of reciprocal degrees of the degrees lying on the cycle grows at most linearly with the number of vertices. This gives one a reason to believe that the minimizing graphs will tend to have many vertices of degree 2, while the maximizing ones will tend to have the contributing degrees concentrated in a small number of vertices, maybe just in one. In addition, for the minimizing graphs, the cycle should be short, hence forcing the vertices of degree 2 into long path(s). The role of the vertices of degree one is not immediately clear. In order to elucidate the structure of extremal graphs, we first establish some auxiliary results.

Proposition 3.4. *Let $U_{n,k}$ be a unicyclic graphs whose unique cycle has length k and is induced by vertices $v_1, \ldots, v_k$, where $k < n - 1$. If more than one of vertices $v_1, \ldots, v_k$ has the degree greater than 2, then there is another graph $U'_{n,k}$ on the same number of vertices and with the same girth such that $\tau(L(U'_{n,k})) > \tau(L(U_{n,k}))$.*

Proof. Let v_i and v_j be two vertices lying on C_k with degrees d_i and d_j, respectively. If both d_i and d_j are greater than 2, it means that there are two non-empty trees, denote them by T_i and T_j, which are rooted at v_i and v_j, respectively. What happens with $\tau(U_{n,k})$ if we uproot the tree T_i from v_i and transplant it to v_j? We claim that the graph $U'_{n,k}$ obtained by this transplantation has a greater number of spanning trees in its line graph. The new degree of v_i becomes 2, the new degree of v_j becomes $d_i + d_j - 2$, and the degrees of all other vertices remain unchanged. Hence, in order to asses the effect of the transplantation on $\tau(L(U_{n,k}))$, we must compare only two pairs of contributions.

The first one is the pair of contributions to the sum of inverse degrees. We claim that the new v_i and v_j contribute more to $\tau(L(U'_{n,k}))$ than the old ones contribute to $\tau(L(U_{n,k}))$. In other words, we claim that $\frac{1}{2} + \frac{1}{d_i+d_j-2} > \frac{1}{d_i} + \frac{1}{d_j}$. Indeed, by considering the function $f(x,y) = \frac{1}{x+y-2} + \frac{1}{2} - \frac{1}{x} - \frac{1}{y}$ and by rewriting it as $f(x,y) = \frac{(x-2)(y-2)(x+y)}{2xy(x+y-2)}$, one can notice that all its factors are positive on $(2,\infty) \times (2,\infty)$. Hence $f(d_i,d_j) > 0$, since the degrees d_i, d_j are greater than 2 in $U_{n,k}$.

It remains to compare the contributions of the old and new v_i and v_j to the product in the right-hand side of Proposition 3.3. To that end, we consider the function $f(x,y) = \frac{(x+y-2)^{x+y-4}}{x^{x-2}y^{y-2}}$. It can be rearranged as

$$f(x,y) = \frac{(x+y-2)^{x-2}}{x^{x-2}} \frac{(x+y-2)^{y-2}}{y^{y-2}} = \left(\frac{x+y-2}{x}\right)^{x-2} \left(\frac{x+y-2}{y}\right)^{y-2}.$$

Clearly, $f(x,y) > 1$ for all $(x,y) \in (2,\infty) \times (2,\infty)$, since each fraction is greater than one and both exponents are positive. By plugging in $x = d_i$, $y = d_j$ we immediately obtain that $(d_i + d_j - 2)^{(d_i+d_j-4)} > {d_i}^{d_i-2}{d_j}^{d_j-2}$. Hence, the contributions of the new degrees of v_i and v_j to both parts of the formula of Proposition 3.3 to $\tau(L(U'_{n,k}))$ exceed the corresponding contributions to $\tau(L(U_{n,k}))$, and our claim follows. ■

Proposition 3.4 implies that in any unicyclic graph maximizing the number of spanning trees in its line graph, all trees must be rooted in the same vertex of its unique cycle. It remains to examine the structure of that tree and also to consider the minimizing case.

Motivated by our previous discussion on the structure of extremal graphs, we consider two special unicyclic graphs on n vertices with the unique cycle of length k. In order to rule out the trivial case, we assume $k < n$, forcing the assumption $n \geq 4$, unless stated otherwise. The first, $CP(n,k)$, is obtained by attaching a path of length $n-k$ to one vertex of C_k. The second, $CS(n,k)$, is obtained by attaching $n-k$ vertices of degree one to the same vertex of C_k. Those graphs are shown in Figure 1. The complexities of their respective line graphs

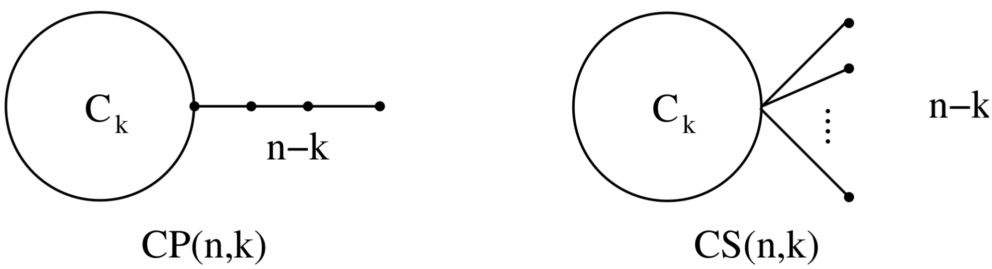

Figure 1: The extremal unicyclic graphs on n vertices with the girth k.

are readily computed from Proposition 3.3 as $\tau(L(CP(n,k))) = 3k-1$ and $\tau(L(CS(n,k))) = (n-k+2)^{n-k-1}\,[n(k-1)+k(3-k)]$. Notice that the first one is increasing, while the other is decreasing when considered as functions of k. In our next result, we show that the two graphs we just introduced bracket all other unicyclic graphs with the same girth.

Proposition 3.5. *Let $U_{n,k}$ be a unicyclic graph on $n \geq 4$ vertices with girth $k < n$. Then*

$$\tau(L(CP(n,k))) \leq \tau(L(U_{n,k})) \leq \tau(L(CS(n,k))),$$

with the left inequality if and only if $U_{n,k} \cong CP(n,k)$ and the right inequality if and only if $U_{n,k} \cong CS(n,k)$.

Proof. We first look at the lower bound. Again, let us suppose that a tree T_i is rooted at each vertex v_i of the unique cycle C_k of $U_{n,k}$, with some trees being, possibly, empty. If $k = n-1$, there is only one such graph and the claim is trivially valid. Suppose, hence, that $k \leq n-2$. It is clear that the vertices of degree 2 in trees do not contribute to $\tau(L(U_{n,k}))$. (The vertices of degree 2 in C_k, if any, contribute by participating in the sum of inverse degrees.) Take a tree T_i rooted at v_i. If T_i is the only non-empty tree, and if it has only one leaf, then T_i is a path and hence $U_{n,k} = CP(n,k)$, the claim is, again, trivially valid. Hence we may assume that T_i has at least two leaves. Fix two of them, w_i and w_i', and transplant w_i' to w_i so that the degree of w_i becomes 2. If w_i' was not adjacent to v_i, this operation cannot increase $\tau(L(U_{n,k}))$; it can decrease it, though, if the only neighbor of w_i' in T_i had a degree greater than 2. In that way, we can transplant all leaves of T_i not adjacent to v_i to a path growing from one of its original leaves without increasing $\tau(L(U_{n,k}))$. In the same way, we can transplant all other leaves from other non-empty trees, if any, not adjacent to the vertices of the unique cycle. What happens if we transplant a leaf adjacent to a vertex on C_k, say, to v_j? Since $d_j \geq 3$, the contribution of v_j will decrease from $d_j^{\,d_j-2}$ to $(d_j-1)^{\,d_j-3}$. On the other hand, the contribution of v_j to the sum of reciprocal degrees will increase from $1/d_j$ to $1/(d_j-1)$. This increase, however, is small, by a factor less than one, and it is more than offset by the decrease which is by a factor at least three. So, the total effect of such transplantations is decreasing, and they can be continued until all vertices not in C_k are in a single path, necessarily having $n-k$ vertices. Hence, the left inequality is established.

In order to establish the upper bound, suppose that at least two trees, T_i and T_j, are non-empty. From Proposition 3.4 we know that such graph cannot maximize $\tau(L(U_{n,k}))$. Hence any maximizing graph must have exactly one non-empty tree. Let T_i be that tree. If all non-root vertices of T_i are leaves, then $U_{n,k} = CS(n,k)$, and we are done. If not, let us take any non-root vertex z of T_i of the largest degree, and transplant the sub-tree rooted in z_i to v_i. It means that z becomes a leaf, and all its neighbors, except the one on the unique path between v_i and z, become neighbors of v_i. We need to consider the ratio of the contributions of z and v_i to $\tau(L(U_{n,k}))$ after and before the transplanting operation. The task is even easier than in Proposition 3.4, since the ratio

$$\frac{(d_{v_i}+d_z-1)^{d_{v_i}+d_z-3}}{d_{v_i}^{d_{v_i}-2}\,d_z^{d_z-2}} = \left(\frac{d_{v_i}+d_z-1}{d_{v_i}}\right)^{d_{v_i}-2}\left(\frac{d_{v_i}+d_z-1}{d_z}\right)^{d_z-2}(d_{v_i}+d_z-1),$$

is clearly greater than one, since all factors exceed one. Moreover, the last factor more than offset the small decrease in the sum of reciprocal degrees which falls from $\frac{k-1}{2}+\frac{1}{d_{v_i}}$ to $\frac{k-1}{2}+\frac{1}{d_{v_i}+d_z-1}$. Hence the total effect of the transplantation is an increase in $\tau(L(U_{n,k}))$. The process can be continued until all non-leaves of T_i have been transplanted to v_i. ■

We can now formulate our main result.

Theorem 3.6. *Let U_n be a unicyclic graph on n vertices and $L(U_n)$ its line graph. Then*

$$\min\{n, 8\} \leq \tau(L(U_n)) \leq 2n(n-1)^{n-4}.$$

The right inequality is attained if and only if $U_n \cong CS(n,3)$. The left inequality is attained for C_n for $3 \leq n \leq 7$, for C_8 and $CP(8,3)$ if $n = 8$, and if and only if $U_n \cong CP(n,3)$ for $n > 8$.

For $n > 8$, Theorem 3.6 follows by noticing that the lower bound of Proposition 3.5 is increasing, and the upper bound is a decreasing function of the cycle length k. For the remaining cases, $3 \leq n \leq 8$, the upper bound follows from Proposition 3.5, while the lower bound is obtained by the fact that the line graph of a cycle is isomorphic to the cycle and formula $\tau(C_n) = n$. It is interesting to notice that the lower bound is independent of n, except for $3 \leq n \leq 8$.

4 Concluding remarks

The number of spanning trees is often used as a measure of the complexity of graphs. In many cases it can be efficiently computed, but only rarely is it given by simple closed formulas in terms of some basic graph parameters. In this paper, we have shown how some explicit formulas for the number of spanning trees in line graphs can be interpreted in terms of multiplicative Zagreb indices. This enabled us to determine the unicyclic graphs whose line graphs have the smallest and the largest number of spanning trees. It would be interesting to explore whether the presented approach could be extended also to the graphs with higher cyclomatic numbers and to graphs in which cycles are well separated. We believe that the corresponding results could be obtained at least for the bicyclic graphs, and that they could be extended to the class of cactus graphs.

With some additional effort, Proposition 3.3 could yield other unicyclic graphs whose line graphs have complexities close to the extremal ones. We invite the reader to verify that the second largest complexity of the line graph of a unicyclic graph on n vertices is obtained for a cycle of length 3 with $n-4$ leaves attached to one of its vertices, and a single leaf attached to another vertex. Also, the next-to-smallest value of 11 is obtained (for large enough n) for the line graph of $CP(n,4)$, independent of n. We leave it to the interested reader to investigate the effects of various ways of attaching leaves to short cycles in order to obtain other close-to-maximum values of $\tau(L(U_n))$.

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