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Open quipus with the same Wiener index as their quadratic line graph☆

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ABSTRACT

An open quipu is a tree constructed by attaching a pendant path to every internal vertex of a path. We show that the graph equation $W(L^2(T)) = W(T)$ has infinitely many non-homeomorphic solutions among open quipus. Here $W(G)$ and $L(G)$ denote the Wiener index and the line graph of G respectively. This gives a positive answer to the 2004 problem of Dobrynin and Mel'nikov on the existence of solutions with arbitrarily large number of arbitrarily long pendant paths, and disproves the 2014 conjecture of Knor and Škrekovski.

1. Introduction

The Wiener index of a graph is the sum of distances between all pairs of its vertices. It was suggested as a structural descriptor of acyclic organic molecules by Harry Wiener in 1947 [38], due to its high correlation with the paraffin boiling points. Its relations to several further properties of organic molecules were subsequently discovered, and it is now widely used by chemists in quantitative structure-activity relationship studies. See, e.g., [10] for an overview of applications of Wiener index, and [40] for an extensive survey. Further recent developments can be found in [1,17,20,27,31,35]. Wiener index attracted attention of mathematicians in the late 1970s when it was introduced in graph theory under the names distance of a graph and transmission of a graph [16,34,36], and is further studied in the form of average distance of graphs and networks [7,8]. In [38] Wiener also proposed the so-called Wiener polarity index, that recently found interest among researchers [15,32,33].

The line graph $L(G)$ of a graph G has edges of G as its vertices, and two vertices of $L(G)$ are adjacent if they have a common vertex as edges of G. The iterated line graphs $L^n(G)$ where n is a nonnegative integer are recursively defined by $L^n(G) = L(L^{n-1}(G))$, where $L^0(G) = G$. The size of $L^n(G)$ rapidly increases for most graphs, reflecting the branching (hence the structural complexity) of G. An accepted opinion in the mathematical chemistry community [13] is that it may be of interest to characterize molecular graphs by means of structural descriptors calculated for their derived structures. Iterated line graphs serve as a good example of derived structures, since their invariants have been already used for characterizing branching of acyclic molecular graphs [3], establishing partial order among isomeric structures [4], evaluating structural complexity of molecular graphs [18] and designing novel structural descriptors [19].

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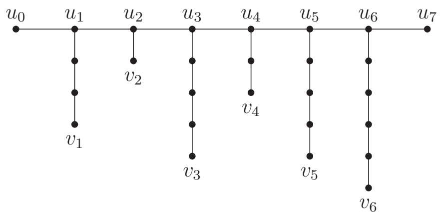

Fig. 1. The open quipu $Q(3,1,4,2,4,5)$.

A problem that has raised considerable interest among graph theorists is the equation

$$W(L^i(T)) = W(T) \tag{1}$$

where T is a tree and i is a positive integer. For $i = 1$, this equation has no nontrivial solutions, due to the seminal result of Buckley:

Theorem 1. *[5] For every tree T holds $W(L(T)) = W(T) - \binom{n}{2}$.*

The case $i \geq 3$ has been fully resolved recently in a series of papers [2,21–26] where it was shown that, for $i \geq 3$, Eq. (1) has a solution among nontrivial trees if and only if $i = 3$ and T is a particular tree $H_{a,b,c}$ whose description follows: $H_{a,b,c}$ is a tree on $a+b+c+4$ vertices, out of which two vertices have degree 3, four vertices have degree 1, and the remaining vertices have degree 2. The two vertices of degree 3 are connected by a path of length 2. There are two pendant paths of lengths a and b attached to one vertex of degree 3, and two pendant paths of lengths c and 1 attached to the other vertex of degree 3. Then

$$W(L^3(H_{a,b,c})) = W(H_{a,b,c})$$

if and only if there exist $j, k \in \mathbb{Z}$ such that

$$\begin{aligned} a &= 128 + 3j^2 + 3k^2 - 3jk + j, \\ b &= 128 + 3j^2 + 3k^2 - 3jk + k, \\ c &= 128 + 3j^2 + 3k^2 - 3jk + j + k. \end{aligned}$$

The smallest such tree has 388 vertices, which is way out of reach of the brute force power of modern day personal computers. Note that all these solutions $H_{a,b,c}$ are homeomorphic to the tree H with degree sequence (3, 3, 1, 1, 1, 1).

To complete the study of Eq. (1) it remains to resolve the case $i = 2$. Small trees satisfying

$$W(L^2(T)) = W(T) \tag{2}$$

have been enumerated in [10] (up to 17 vertices) and [11] (up to 26 vertices). Constructions of infinite families of trees satisfying Eq. (2) are given by Dobrynin and Mel'nikov [11–14] and by Knor and Škrekovski [28]. However, every known example of trees satisfying this equation has at most four vertices of degree ≥ 3 and at most four paths whose lengths can be arbitrarily large. These findings motivated Dobrynin and Mel'nikov to pose the following problem.

Problem 2. *[11] Find an infinite family $\mathcal{F}$ of trees T satisfying Eq. (2) such that for arbitrary $n, m \in \mathbb{N}$ the family $\mathcal{F}$ contains a tree T with at least n pendant paths each having length at least m.*

Let $\mathcal{T}$ be the set of trees that have no vertices of degree 2 and such that $T' \in \mathcal{T}$ if and only if there exists a tree T homeomorphic to T' that satisfies Eq. (2). Knor and Škrekovski pose the following conjecture.

Conjecture 3. *[28] $\mathcal{T}$ is a finite set.*

We resolve both Problem 2 and Conjecture 3. Since both questions are related to the existence of trees with arbitrarily large number of vertices of degree at least 3 and arbitrarily long pendant paths, we opt to search for solutions of Eq. (2) among trees having the form depicted in Fig. 1, as they are well suited for both these requirements. These trees, which have maximum degree three and in which the vertices of degree three induce a path, are called open quipus by Roo and Neumaier [39]. They are extensively studied in the problem of characterizing graphs with a given diameter and minimal spectral radius [6,9,29,30,37,41], as they represent examples of graphs whose spectral radius is small—at most $\frac{3}{2}\sqrt{2}$ (other such graphs are closed quipus, in which vertices of degree three induce a cycle, and a dagger, obtained from a path by adding three pendant vertices at one of its end vertices [39]). Our computer-generated catalogs show that Eq. (2) has an abundance of solutions among open quipus, and careful mining of these solutions enabled us to prove the following theorem which positively answers Problem 2 and disproves Conjecture 3.

Theorem 4. *For each natural number $t \geq 5$, there exists an open quipu Q satisfying $W(L^2(Q)) = W(Q)$ such that Q contains $12t^2 - 201$ vertices of degree three and each pendant path of Q other than two pendant edges, has length either $8t^2 - 136$ or $8t^2 - 135$.*