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Contraction Formulas for the Kirchhoff and Wiener Indices

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Abstract

We relate the Kirchhoff index with some other metrized graph invariants. We establish several contraction formulas for the Kirchhoff index. We use these contraction formulas and certain edge densities to give new upper and lower bounds to the Kirchhoff index for any connected graph. As an another application of our contraction formulas when the graph is a tree, we derive new formulas as well as previously known formulas for the Wiener index with new proofs.

1 Introduction

On a metrized graph Γ with set of vertices $V(\Gamma)$ and resistance function $r(x,y)$, the Kirchhoff index $Kf(\Gamma)$ is defined as follows:

$$Kf(\Gamma) = \frac{1}{2} \sum_{p,\, q \in V(\Gamma)} r(p,q) \ .$$

For the distance function $d(x,y)$ on Γ, the Wiener index $W(\Gamma)$ is defined as:

$$W(\Gamma) = \frac{1}{2} \sum_{p,\, q \in V(\Gamma)} d(p,q) \ .$$

These definitions of $Kf(\Gamma)$ and $W(\Gamma)$ on a metrized graph Γ agree with their usual definitions on a graph (see [15] and [13], respectively). A metrized graph Γ is a finite connected graph equipped with a distinguished parametrization of each of its edges. One can consider Γ as a one-dimensional manifold except at finitely many branch points, where it looks locally like an n-pointed star. A metrized graph Γ can have multiple edges and self-loops. Next, we give a summary of the results we obtained in this paper.

In §2, we give a short review of metrized graphs and some notations we use.

In §3, we briefly describe the voltage and the resistance functions on a metrized graph. We set notations concerning some specific values of these functions and recall some basic results that we use.

In §4, we improve Kirchhoff index formulas we obtained in [7]. Then we extend the contraction formulas obtained in [6] to bridgeless graphs. Using these results, we give a new contraction formula for the Kirchhoff index that involves another graph invariant $y(\Gamma)$ (see Equation (2) for the definition of $y(\Gamma)$ and Theorem 4.5 for the contraction formula). This enables us giving lower and upper bounds to the Kirchhoff index in terms of $y(\Gamma)$, and more importantly this contraction formula of the Kirchoff index can be applied successively (see Theorem 4.12). Since the Kirchhoff index of Γ is closely related to the trace of the pseudo inverse of the discrete Laplacian matrix of Γ when Γ has no self loops and multiple edges, the contraction formulas we derived for the Kirchhoff index have equivalent forms in terms of the related traces (e.g., see Theorem 4.18 below).

In §5, we use the contraction formulas we derived to give upper and lower bounds to the Kirchhoff index for connected graphs. This is given in Theorem 1.1 below.

Let G be a finite connected graph with set of vertices V. Suppose $\{V_1, V_2\}$ be a partition of V, i.e., V_1 and V_2 are two disjoint nonempty subsets of V such that $V = V_1 \cup V_2$. We call the partition $\{V_1, V_2\}$ be admissible if both of the induced subgraphs $G[V_1]$ and $G[V_2]$ are connected. If one takes a spanning tree T of G, each edge e_T of T determines an admissible partition of V by considering V_1 as the vertices on one side of e_T and V_2 as the vertices on the other side. Let $E(V_1, V_2)$ be the set of edges of G connecting a vertex in V_1 with a vertex in V_2. We define the edge density $d(V_1, V_2)$ of an admissible partition $\{V_1, V_2\}$ as follows:

$$d(V_1, V_2) = \frac{|E(V_1, V_2)|}{|V_1| \cdot |V_2|} \ . \tag{1}$$

For $S = \big\{ d(V_1, V_2) \mid \{V_1, V_2\} \text{ is an admissible partition of } V \big\}$, we set

$$d_{\min} = \min S, \qquad \text{and} \qquad d_{\max} = \max S \ .$$

Theorem 1.1. *(See Theorem 5.1 and Corollary 5.2) Let G be a finite connected graph with $v \geq 2$ vertices and e edges, and let each edge of G have length* 1*. Then we have*

$$\frac{(v-1)^2}{e-v+2} \leq \frac{v-1}{d_{\max}} \leq Kf(G) \leq \frac{v-1}{d_{min}} \leq \frac{v^2(v-1)}{4\Lambda} \, ,$$

where Λ *is the edge connectivity of* G.

Note that the upper bound $Kf(G) \leq \frac{v^2(v-1)}{4\Lambda}$ was given in [7, Theorem 1.3] for regular graphs. Here we have it for any graph.

We deal with tree metrized graphs in §6. Note that the Kirchhoff index is the same as the Wiener index for a tree graph. We restate the results we derived for the Kirchhoff index in §4 for a tree graph. In this way, we obtain contraction formulas for the Wiener index of a tree graph. Moreover, we obtain new formulas, given in Theorem 6.3 and Theorem 6.6 below, for the Wiener index. Our approach enables us to give new proofs of some previously known formulas, Theorem 6.2 and Theorem 6.9, for the Wiener index. Then we give various examples that apply our formulas to compute Wiener indices. At the end of §6, we state two problems. Solution to any of them will be a new proof of a conjecture about the Wiener index (see Theorem 6.10 below). One can consult [18] for possible uses of these formulas about the Wiener index and the use of the Wiener index.

Note that there is a one-to-one correspondence between metrized graphs and certain equivalence class of finite connected weighted graphs in which the weight of an edge is the reciprocal of its length [2, Lemma 2.2]. We can also view such a graph as a resistive electrical network in which the resistance of each edge is the same as its length. The identities that we establish for metrized graphs in this paper are also valid for electrical networks, and they have equivalent forms for corresponding weighted graphs.

2 Metrized Graphs

In this section, we give a brief review of metrized graphs to make this paper self contained as much as possible.

"Metrized graph" as a term was introduced by Rumely [19], and developed further in [3] and [23]. Here is a rigorous definition of a metrized graph:

Definition. [23] [2, Definition 2.1] A metrized graph Γ is a compact, connected metric space such that for each $p \in \Gamma$, there exist a radius $r_p > 0$ and an integer $\upsilon(p) \geq 1$ such that p has a neighborhood $V_p(r_p)$ isometric to the star-shaped set

$$S(\upsilon(p), r_p) \;=\; \{z \in \mathbb{C} : z = te^{k \cdot 2\pi i/\upsilon(p)} \text{ for some } 0 \leq t < r_p \text{ and some } k \in \mathbb{Z}\},$$

equipped with the path metric.

A leisurely survey on metrized graphs can be found in [1]. Following [2], we consider a metrized graph as an analytic object, not just a combinatorial one. We can intuitively describe metrized graphs as follows:

A metrized graph Γ is a finite connected graph equipped with a distinguished parametrization of each of its edges. Thus, a metrized graph Γ can have multiple edges and self-loops.

Metrized graphs are also known in the literature as networks, metric graphs, and quantum graphs. For a discussion about the connections and differences about these notions, one can see [2, Page 226 and §1.9] and the papers cited therein.

For any given $p \in \Gamma$, the number $\upsilon(p)$ of directions emanating from p will be called the *valence* of p. By definition, there can be only finitely many $p \in \Gamma$ with $\upsilon(p) \neq 2$.

For a metrized graph Γ, we denote a vertex set for Γ by $V(\Gamma)$. We require that $V(\Gamma)$ be finite and non-empty and that $p \in V(\Gamma)$ for each $p \in \Gamma$ if $\upsilon(p) \neq 2$.

For a given metrized graph Γ with vertex set $V(\Gamma)$, the set of edges of Γ is the set of closed line segments with end points in $V(\Gamma)$. We will denote the set of edges of Γ by $E(\Gamma)$. However, if e_i is an edge, by $\Gamma - e_i$ we mean the graph obtained by deleting the *interior* of e_i.

We denote the length of an edge $e_i \in E(\Gamma)$ by L_i, which represents a positive real number. The total length of Γ, which is denoted by $\ell(\Gamma)$, is given by $\ell(\Gamma) = \sum_{i=1}^{e} L_i$.

For a given metrized graph Γ, it is possible to enlarge the vertex set $V(\Gamma)$ by considering additional valence 2 points as vertices. However, this process of enlarging the vertex set does not change the total length of Γ. Figure 1 illustrates an example.

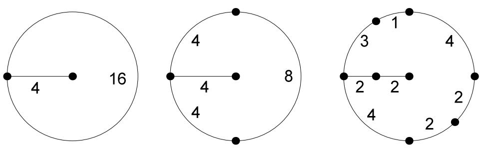

Figure 1: A metrized graph Γ with three different graph models.

The connections between metrized graphs and finite weighted graphs are explicitly discussed in [2, §2].

We use the notation $\overline{\Gamma}_i$ for the graph obtained by contracting the i-th edge e_i of a given metrized graph Γ to its end points. If $e_i \in \Gamma$ has end points p_i and q_i, then in $\overline{\Gamma}_i$, these points become identical, i.e., $p_i = q_i$. If p is an end point of an edge e_i in Γ, then by p in $V(\overline{\Gamma}_i)$ we mean the vertex, in $V(\overline{\Gamma}_i)$, that p is contracted into.

3 Resistance Function $r(x, y)$

In this section, we briefly describe the resistance and the voltage functions on a metrized graph Γ. We make a review of basic facts about these functions and then set notations that we use in the rest of the paper.

For any x, y, z in Γ, the voltage function $j_z(x, y)$ on a metrized graph Γ is a symmetric function in x and y, which satisfies $j_x(x, y) = 0$ and $j_z(x, y) \geq 0$ for all x, y, z in Γ. For each vertex set $V(\Gamma)$, $j_z(x, y)$ is continuous on Γ as a function of all three variables. For fixed z and y it has the following physical interpretation: If Γ is viewed as a resistive electric circuit with terminals at z and y, with the resistance in each edge given by its length, then $j_z(x, y)$ is the voltage difference between x and z, when unit current enters at y and exits at z (with reference voltage 0 at z).

The effective resistance between two points x, y of a metrized graph Γ is given by $r(x, y) = j_y(x, x)$, where $r(x, y)$ is the resistance function on Γ. The resistance function inherits certain properties of the voltage function. For any x, y in Γ, $r(x, y)$ on Γ is a symmetric function in x and y, and it satisfies $r(x, x) = 0$. For each vertex set $V(\Gamma)$, $r(x, y)$ is continuous on Γ as a function of two variables and $r(x, y) \geq 0$ for all x, y in Γ. If a metrized graph Γ is viewed as a resistive electric circuit with terminals at x and y, with the resistance in each edge given by its length, then $r(x, y)$ is the effective resistance between x and y when unit current enters at y and exits at x.

Note that these definitions of the voltage and the resistance functions on a metrized graph Γ agree with the definitions on each of the graph model of Γ. Here by a graph model of Γ we mean the corresponding finite weighted graph associated to the chosen vertex set of Γ. Thus, for any points x, y and z in Γ the values $r(x, y)$ and $j_z(x, y)$ agree with the values on any chosen graph model of Γ whose vertex set contains these three points. These functions on a graph are considered as functions with a discrete set as the domain, namely the vertex set. However, we have the continuous version of these functions on a metrized graph.

The proofs of the facts mentioned above can be found in [3] and [2, Sections 1.5 and 6]. The voltage function $j_z(x, y)$ and the resistance function $r(x, y)$ are also studied in [1].

We will denote by R_i the resistance between the end points of an edge e_i of a graph Γ when the interior of the edge e_i is deleted from Γ.

Let Γ be a metrized graph with $p \in V(\Gamma)$, and let $e_i \in E(\Gamma)$ having end points p_i and q_i. If $\Gamma - e_i$ is connected, then Γ can be transformed to the graph in Figure 2 by circuit reductions (see [4, Page 642]). More details on this fact can be found in the articles [3] and [5, Section 2]. Note that in Figure 2, we have $R_{a_i,p} = \hat{j}_{p_i}(p, q_i)$, $R_{b_i,p} = \hat{j}_{q_i}(p, p_i)$, $R_{c_i,p} = \hat{j}_p(p_i, q_i)$, where $\hat{j}_x(y, z)$ is the voltage function in $\Gamma - e_i$. We have $R_{a_i,p} + R_{b_i,p} = R_i$ for each $p \in \Gamma$.

Remark 3.1. *If $\Gamma - e_i$ is not connected, firstly we set $R_{b_i,p} = R_i$ and $R_{a_i,p} = 0$ if p belongs to the component of $\Gamma - e_i$ containing p_i, and we set $R_{a_i,p} = R_i$ and $R_{b_i,p} = 0$ if p belongs to the component of $\Gamma - e_i$ containing q_i. Secondly, we mean $R_i \longrightarrow \infty$ in any expression that we use R_i.*

We will use these notations for the rest of the paper. Next, we recall a basic identity concerning these values:

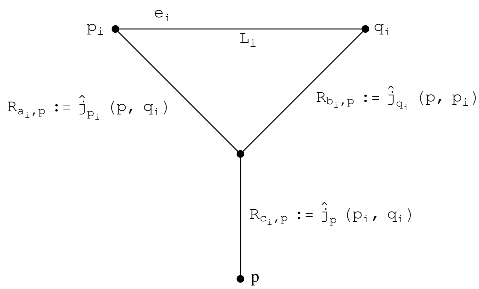

Figure 2: Circuit reduction of Γ with reference to an edge e_i and a point p.

Lemma 3.2. *[5, Lemma 2.11] For any p and q in $V(\Gamma)$,*

$$\sum_{e_i \in E(\Gamma)} \frac{L_i(R_{a_i,p} - R_{b_i,p})^2}{(L_i + R_i)^2} = \sum_{e_i \in E(\Gamma)} \frac{L_i(R_{a_i,q} - R_{b_i,q})^2}{(L_i + R_i)^2}.$$

In the rest of the paper, for any metrized graph Γ and a fixed vertex $p \in V(\Gamma)$ we will use the following notations, which we first defined in [8] and used also in [7]:

$$\begin{aligned} y(\Gamma) &= \frac{1}{4} \sum_{e_i \in E(\Gamma)} \frac{L_i R_i^2}{(L_i + R_i)^2} + \frac{3}{4} \sum_{e_i \in E(\Gamma)} \frac{L_i(R_{a_i,p} - R_{b_i,p})^2}{(L_i + R_i)^2}, \\ x(\Gamma) &= \sum_{e_i \in E(\Gamma)} \frac{L_i^2 R_i}{(L_i + R_i)^2} + \frac{3}{4} \sum_{e_i \in E(\Gamma)} \frac{L_i R_i^2}{(L_i + R_i)^2} - \frac{3}{4} \sum_{e_i \in E(\Gamma)} \frac{L_i(R_{a_i,p} - R_{b_i,p})^2}{(L_i + R_i)^2}. \end{aligned} \tag{2}$$

Note that $x(\Gamma)$ and $y(\Gamma)$ do not depend on the choice of the vertex p by Lemma 3.2. In [7], we established connections between the Kirchhoff index of Γ and the invariants $x(\Gamma)$ and $y(\Gamma)$.

When we use $r_\beta(x,y)$, we mean the resistance function in the metrized graph β.

4 Contraction Formulas for the Kirchhoff Index

The Kirchhoff index of a graph Γ, $Kf(\Gamma)$, is defined [15] as follows:

$$Kf(\Gamma) := \frac{1}{2} \sum_{p,\, q \in V(\Gamma)} r(p,q) \ . \tag{3}$$

The following equality was obtained in [7, Page 4038]. It gives a relation between the Kirchhoff index of Γ and the Kirchhoff indexes of $\overline{\Gamma}_i$'s. Although it is a useful formula to understand how the Kirchhoff index changes after edge contractions, we can not use it for successive edge contractions because of some technical problems.

$$(v-2)Kf(\Gamma) = \sum_{e_i \in E(\Gamma)} \frac{R_i}{L_i+R_i} Kf(\overline{\Gamma}_i) + \sum_{e_i \in E(\Gamma)} \frac{R_i}{L_i+R_i} \sum_{p \in V(\overline{\Gamma}_i)} r_{\overline{\Gamma}_i}(p, \overline{p}_i) \ . \tag{4}$$

The idea of tracing the value of a graph invariant after successive edge contractions was successfully applied in [6], where we studied the tau constant as an another graph invariant. We want to utilize this idea for the Kirchhoff index. To do this, we first need various technical results.

The following lemma is to express $r_{\overline{\Gamma}_i}(p, \overline{p}_i)$ in terms of the resistance values on Γ that we are more familiar.

Lemma 4.1. *Let Γ be a metrized graph, and let p be a vertex of Γ. For an edge e_i of Γ with end points p_i and q_i, we have*

$$r(p_i,p) + r(q_i,p) = 2r_{\overline{\Gamma}_i}(p,\overline{p}_i) + \frac{L_iR_i}{L_i+R_i} - 2\frac{L_iR_{a_i,p}R_{b_i,p}}{R_i(L_i+R_i)} \ .$$

Proof. We prove this in two cases.

Case I: e_i is not a bridge.

From [5, Section 2], we have

$$r(p_i,p) = \frac{(L_i+R_{b_i,p})R_{a_i,p}}{L_i+R_i} + R_{c_i,p}, \quad \text{and} \quad r(q_i,p) = \frac{(L_i+R_{a_i,p})R_{b_i,p}}{L_i+R_i} + R_{c_i,p} \ . \tag{5}$$

Thus,

$$r(p_i,p) + r(q_i,p) = \frac{L_iR_i}{L_i+R_i} + 2\frac{R_{a_i,p}R_{b_i,p}}{L_i+R_i} + 2R_{c_i,p} \ . \tag{6}$$

On the other hand, from [8, Equation 17] we have

$$r_{\overline{\Gamma}_i}(p,\overline{p}_i) = \frac{R_{a_i,p}R_{b_i,p}}{R_i} + R_{c_i,p} \ . \tag{7}$$

Thus, the result follows from Equations (6) and (7) in this case.

Case II: e_i is a bridge.

If p belongs to the component of $\Gamma - e_i$ containing p_i, we have $r(p_i,p) + r(q_i,p) = L_i + 2r(p_i,p)$ and $r_{\overline{\Gamma}_i}(p,\overline{p}_i) = r(p_i,p)$.

If p belongs to the component of $\Gamma - e_i$ containing q_i, we have $r(p_i,p) + r(q_i,p) = L_i + 2r(q_i,p)$ and $r_{\overline{\Gamma}_i}(p,\overline{p}_i) = r(q_i,p)$.

Now, we note that $\frac{L_iR_i}{L_i+R_i} \longrightarrow L_i$ and $\frac{L_iR_{a_i,p}R_{b_i,p}}{R_i(L_i+R_i)} \longrightarrow 0$ because of Remark 3.1.

Thus, the result follows in this case, too. ∎

Now, we can substitute the value of $r_{\overline{\Gamma}_i}(p,\overline{p}_i)$ obtained from Lemma 4.1 into the formula given in Equation (4). In this way, we derive a new formula for the Kirchhoff index.

Lemma 4.2. *Let Γ be a metrized graph. We have*

$$\begin{aligned} 2(v-2)Kf(\Gamma) = 2\sum_{e_i \in E(\Gamma)} \frac{R_i}{L_i+R_i} Kf(\overline{\Gamma}_i) + 2v \sum_{e_i \in E(\Gamma)} \frac{L_iR_{a_i,p}R_{b_i,p}}{(L_i+R_i)^2} - v\sum_{e_i \in E(\Gamma)} \frac{L_iR_i^2}{(L_i+R_i)^2} \\ + \sum_{p \in V(\Gamma)} \sum_{e_i \in E(\Gamma)} \frac{R_i}{L_i+R_i}\big(r(p_i,p) + r(q_i,p)\big) \ . \end{aligned}$$

Proof. Since $R_i = R_{a_i,p} + R_{b_i,p}$ for any $p \in V(\Gamma)$, we have

$$\sum_{e_i \in E(\Gamma)} \frac{L_iR_i^2}{(L_i+R_i)^2} = \sum_{e_i \in E(\Gamma)} \frac{L_i(R_{a_i,p} - R_{b_i,p})^2}{(L_i+R_i)^2} + 4\sum_{e_i \in E(\Gamma)} \frac{L_iR_{a_i,p}R_{b_i,p}}{(L_i+R_i)^2} \ . \tag{8}$$

We note that the left hand side of Equation (8) is independent of the choice of the vertex p. Likewise, the first term at the right side of Equation (8) is independent of p because of Lemma 3.2. Therefore,

$$\sum_{e_i \in E(\Gamma)} \frac{L_iR_{a_i,p}R_{b_i,p}}{(L_i+R_i)^2} = \sum_{e_i \in E(\Gamma)} \frac{L_iR_{a_i,q}R_{b_i,q}}{(L_i+R_i)^2}, \qquad \text{for any vertices } p \text{ and } q. \tag{9}$$

Now, we first multiply the equality in Lemma 4.1 by $\frac{R_i}{L_i+R_i}$ and take the summation of the resulting equality over all edges e_i in $E(\Gamma)$. Then we take the summation of the equality obtained over all vertices p in $V(\Gamma)$. Finally, the result follows from Equation (9), Equation (4) and the equality we derived. ∎

Now, our goal is to simplify the formula we obtained in Lemma 4.2. First, we improve a result we derived previously.

The following lemma with the condition that Γ is a bridgeless metrized graph was proved in [8, Lemma 3.10]. We note that this condition is not necessary.

Lemma 4.3. *Let Γ be a metrized graph, and let p_i and q_i be end points of $e_i \in E(\Gamma)$. For any $p \in V(\Gamma)$, we have*

$$\sum_{e_i \in E(\Gamma)} \frac{L_i (R_{a_i,p} - R_{b_i,p})^2}{(L_i + R_i)^2} = \sum_{e_i \in E(\Gamma)} \frac{L_i}{L_i + R_i} \big(r(p_i, p) + r(q_i, p) \big) - \sum_{q \in V(\Gamma)} (\upsilon(q) - 2) r(p, q)$$
$$= 2 \sum_{q \in V(\Gamma)} r(p, q) - \sum_{e_i \in E(\Gamma)} \frac{R_i}{L_i + R_i} \big(r(p_i, p) + r(q_i, p) \big) \ .$$

Proof. The proof is almost the same as the proof of [8, Lemma 3.10]. The only additional work is to use the following facts for edges that are bridges (edges whose removal disconnects the graph). Let $e_i \in E(\Gamma)$ be a bridge, and let $p \in V(\Gamma)$. Suppose $x \in e_i$ is as in

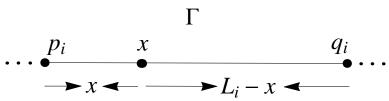

Figure 3: Γ with $x \in e_i$, where e_i is a bridge.

Figure 3 and that e_i has end points p_i and q_i. If p belongs to the component of $\Gamma - e_i$ containing p_i, we have

$$r(p, x) = r(p, p_i) + x, \qquad \frac{d}{dx} r(p, x) = 1, \quad \text{and } r(p, p_i) - r(p, q_i) = -L_i \ . \tag{10}$$

If p belongs to the component of $\Gamma - e_i$ containing q_i, we have

$$r(p, x) = r(p, q_i) + L_i - x, \qquad \frac{d}{dx} r(p, x) = -1 \quad \text{and } r(p, p_i) - r(p, q_i) = L_i \ . \tag{11}$$

Thus, in any case $\frac{d^2}{dx^2} r(p, x) = 0$ if x belongs to a bridge.

We note that [8, Lemma 3.6], [8, Equation (14)] and [8, Proposition 3.9] are valid for metrized graphs with possibly bridges.

If we consider Remark 3.1 along with Equations (10) and (11), the proof of [8, Lemma 3.10] can be extended to the case Γ with bridges. ∎

Lemma 4.3 is crucial for our purposes.

Lemma 4.4. *For any metrized graph* Γ*, we have*

$$4Kf(\Gamma) = v \cdot \sum_{e_i \in E(\Gamma)} \frac{L_i(R_{a_i,p} - R_{b_i,p})^2}{(L_i+R_i)^2} + \sum_{e_i \in E(\Gamma)} \frac{R_i}{L_i+R_i} \sum_{p \in V(\Gamma)} \big(r(p_i,p) + r(q_i,p)\big).$$

Proof. First, we take summation of the second equality in Lemma 4.3 over all vertices $p \in V(\Gamma)$:

$$\sum_{p \in V(\Gamma)} \sum_{e_i \in E(\Gamma)} \frac{L_i(R_{a_i,p} - R_{b_i,p})^2}{(L_i+R_i)^2} = 2 \sum_{p,q \in V(\Gamma)} r(p,q) - \sum_{e_i \in E(\Gamma)} \frac{R_i}{L_i+R_i} \sum_{p \in V(\Gamma)} r(p_i,p) + r(q_i,p).$$

Then the result follows from this equality, Lemma 3.2 and the definition of $Kf(\Gamma)$. ■

After having various technical lemmas, we can state our first main result. It describes the relation between the Kirchhoff index of Γ and the Kirchhoff indexes of each of $\overline{\Gamma}_i$ that are obtained by contraction of $e_i \in E(\Gamma)$:

Theorem 4.5. *Let* Γ *be a metrized graph with* v *vertices. Then we have*

$$(v-4)Kf(\Gamma) = \sum_{e_i \in E(\Gamma)} \frac{R_i}{L_i+R_i} Kf(\overline{\Gamma}_i) - v \cdot y(\Gamma)\ .$$

Proof. We first subtract the equality given in Lemma 4.4 from the equality given in Lemma 4.2. Then the proof follows from Equation (8) and Equation (2). ■

Next, we have another formula for the Kirchhoff index.

Proposition 4.6. *For any metrized graph* Γ *with* v *vertices, we have*

$$2Kf(\Gamma) = v \cdot y(\Gamma) + \sum_{e_i \in E(\Gamma)} \frac{R_i}{L_i+R_i} \sum_{p \in V(\overline{\Gamma}_i)} r_{\overline{\Gamma}_i}(p, \overline{p}_i)\ .$$

Proof. The result is obtained by subtracting the formula in Theorem 4.5 from Equation (4). ■

Note that Theorem 4.5 is more advantageous to work with than Equation (4), because we studied the term $y(\Gamma)$ previously [6] and showed that it has various properties.

Our goal for the rest of this section is to apply the contraction formula given in Theorem 4.5 successively. To do this, we need the contraction formula for $y(\Gamma)$ for any metrized graph Γ (see Theorem 4.9 below). The contraction formula of $y(\Gamma)$ for bridgeless metrized graphs was shown in [6, Theorem 4.12]. First, we need some preparatory work.

The following theorem was given in [7, Theorem 4.8]. Note that we don't need the condition bridgeless as explained in the paragraph before the theorem in that paper (and as its proof shows). That is, we can give [7, Theorem 4.8] with a minor correction in its statement as follows:

Theorem 4.7. *Let Γ be a metrized graph. For any two vertices p and q, we have*

$$(v-2)r(p,q) = \sum_{e_i \in E(\Gamma)} \frac{R_i}{L_i+R_i} r_{\overline{\Gamma}_i}(p,q) \ .$$

Next, we apply Theorem 4.7 to the sum of effective resistances along with all edges. Let

$$r(\Gamma) := \sum_{e_i \in E(\Gamma)} \frac{L_i R_i}{L_i+R_i} \ .$$

Note that $r(p_i,q_i) = \frac{L_i R_i}{L_i+R_i}$ for any edge e_i with end points p_i and q_i.

Theorem 4.8. *Let Γ be a metrized graph. Then we have*

$$(v-2)r(\Gamma) = \sum_{e_i \in E(\Gamma)} \frac{R_i}{L_i+R_i} r(\overline{\Gamma}_i) \ .$$

Proof. Let e_j be an edge with end points p_j and q_j. Applying Theorem 4.7 to the vertices p_j and q_j gives

$$(v-2)r(p_j,q_j) = \sum_{e_i \in E(\Gamma)} \frac{R_i}{L_i+R_i} r_{\overline{\Gamma}_i}(p_j,q_j) \ .$$

where v is the number of vertices in Γ. Now, if we take the summation of above equality over all edges e_j in Γ and use the definition of $r(\Gamma)$, we obtain

$$\begin{aligned}
(v-2)r(\Gamma) &= \sum_{e_i \in E(\Gamma)} \frac{R_i}{L_i+R_i} \sum_{e_j \in E(\Gamma)} r_{\overline{\Gamma}_i}(p_j,q_j) \\
&= \sum_{e_i \in E(\Gamma)} \frac{R_i}{L_i+R_i} \sum_{e_j \in E(\overline{\Gamma}_i)} r_{\overline{\Gamma}_i}(p_j,q_j), \qquad \text{since } r_{\overline{\Gamma}_i}(p_i,q_i) = 0 \ . \\
&= \sum_{e_i \in E(\Gamma)} \frac{R_i}{L_i+R_i} r(\overline{\Gamma}_i) \ .
\end{aligned}$$

This gives what we want to show. ∎

Note that Theorem 4.8 for bridgeless metrized graphs was given in [6, Corollary 4.13]. But we show here that it holds for any metrized graph possibly with bridges.

Similarly, the following theorem for bridgeless metrized graphs was given in [6, Theorem 4.12].

Theorem 4.9. *Let Γ be a metrized graph with v vertices. Then we have*

$$(v-2)x(\Gamma) = \sum_{e_i \in E(\Gamma)} \frac{R_i}{L_i+R_i} x(\overline{\Gamma}_i) , \qquad \textit{and} \quad (v-2)y(\Gamma) = \sum_{e_i \in E(\Gamma)} \frac{R_i}{L_i+R_i} y(\overline{\Gamma}_i) \ .$$

Proof. Let $B(\Gamma) = \{e_{i_1}, e_{i_2}, \dots, e_{i_t}\}$ be the set of bridges in Γ. Let β be the metrized graph obtained from Γ by contracting all bridges in Γ.

We first note that if e_i is a bridge, using Remark 3.1 we obtain $\frac{L_i^2 R_i}{(L_i+R_i)^2} \longrightarrow 0$, $\frac{L_i R_i^2}{(L_i+R_i)^2} \longrightarrow L_i$ and $\frac{L_i(R_{a_i,p}-R_{b_i,p})^2}{(L_i+R_i)^2} \longrightarrow L_i$. Therefore, considering the definition of $x(\Gamma)$ in Equation (2) we conclude that bridges in Γ does not contribute to $x(\Gamma)$, so $x(\Gamma) = x(\beta)$. Moreover, $R_j(\Gamma) = R_j(\beta)$ if e_j is not a bridge. Hence,

$$\begin{aligned} &x(\Gamma) = x(\overline{\Gamma}_i) \quad \text{when } e_i \text{ is a bridge, and so } x(\overline{\Gamma}_i) = x(\beta). \\ &x(\overline{\Gamma}_i) = x(\overline{\beta}_i) \quad \text{when } e_i \text{ is not a bridge.} \end{aligned} \tag{12}$$

We use Equation (12) and Remark 3.1 in the second equality below:

$$\begin{aligned} \sum_{e_i \in E(\Gamma)} \frac{R_i}{L_i+R_i} x(\overline{\Gamma}_i) &= \sum_{e_i \in E(\Gamma)-B(\Gamma)} \frac{R_i}{L_i+R_i} x(\overline{\Gamma}_i) + \sum_{e_i \in B(\Gamma)} \frac{R_i}{L_i+R_i} x(\overline{\Gamma}_i) \\ &= \sum_{e_i \in E(\Gamma)-B(\Gamma)} \frac{R_i(\beta)}{L_i+R_i(\beta)} x(\overline{\beta}_i) + \sum_{e_i \in B(\Gamma)} x(\beta), \\ &= (v-t-2)x(\beta) + t \cdot x(\beta), \qquad \text{using [6, Theorem 4.12] for } \beta. \\ &= (v-2)x(\Gamma), \qquad \text{since } x(\Gamma) = x(\beta). \end{aligned} \tag{13}$$

This proves the first equality in the theorem. Next, we prove the second equality. We first note that $r(\Gamma) = x(\Gamma) + y(\Gamma)$ for any metrized graph Γ.

On one hand, by Theorem 4.8 we have

$$(v-2)r(\Gamma) = \sum_{e_i \in E(\Gamma)} \frac{R_i}{L_i+R_i} r(\overline{\Gamma}_i) = \sum_{e_i \in E(\Gamma)} \frac{R_i}{L_i+R_i} \big(x(\overline{\Gamma}_i) + y(\overline{\Gamma}_i)\big). \tag{14}$$

On the other hand, by the first equality that we just proved for $x(\Gamma)$

$$(v-2)r(\Gamma) = (v-2)x(\Gamma) + (v-2)y(\Gamma) = (v-2)y(\Gamma) + \sum_{e_i \in E(\Gamma)} \frac{R_i}{L_i+R_i} x(\overline{\Gamma}_i).$$

Thus, the second equality in the theorem follows from this equality and Equation (14).

■

When the number of vertices is 2 or 3, we know the exact relation between $Kf(\Gamma)$ and $y(\Gamma)$.

Corollary 4.10. *For any metrized graph Γ with v vertices we have*

$$Kf(\Gamma) = y(\Gamma) \quad \textit{if} \quad v = 2, \quad \textit{and} \quad Kf(\Gamma) = 2y(\Gamma) \quad \textit{if} \quad v = 3.$$

Proof. When $v = 2$, $\overline{\Gamma}_i$ has only one vertex. In this case, $Kf(\overline{\Gamma}_i) = 0$ for each edge e_i. Then Theorem 4.5 gives that $Kf(\Gamma) = y(\Gamma)$.

When $v = 3$, $\overline{\Gamma}_i$ has two vertices, so we have $Kf(\overline{\Gamma}_i) = y(\overline{\Gamma}_i)$ by the first equality. Thus, Theorem 4.5 gives

$$-Kf(\Gamma) = \sum_{e_i \in E(\Gamma)} \frac{R_i}{L_i + R_i} Kf(\overline{\Gamma}_i) - 3 \cdot y(\Gamma) = \sum_{e_i \in E(\Gamma)} \frac{R_i}{L_i + R_i} y(\overline{\Gamma}_i) - 3 \cdot y(\Gamma) = -2y(\Gamma),$$

where the last equality follows from Theorem 4.9. This completes the proof. ■

For any integer $1 \leq k \leq v - 2$, if an edge e_{i_k} is not a self loop in $\overline{\Gamma}_{i_1,i_2,\ldots,i_{k-1}}$, then $\#(V(\overline{\Gamma}_{i_1,i_2,\ldots,i_k})) = \#(V(\overline{\Gamma}_{i_1,i_2,\ldots,i_{k-1}})) - 1$. We call $\overline{\Gamma}_{i_1,i_2,\ldots,i_k}$ be an *admissible contraction* of Γ, if it is obtained from Γ by contracting edges with distinct end points at each step. We have $\#(V(\overline{\Gamma}_{i_1,i_2,\ldots,i_k})) = v - k$ iff $V(\overline{\Gamma}_{i_1,i_2,\ldots,i_k})$ is an admissible contraction of Γ. Note that we have $\frac{R_i}{L_i+R_i} = 0$ for a self loop, so contraction of self loops can be neglected in contraction identities. Therefore, we restrict ourselves to the admissible contractions only.

Now, we successively apply the contraction identity given in Theorem 4.9 as follows:

Theorem 4.11. *Let Γ be a metrized graph with $v \geq 3$ vertices, and let k be an integer with $1 \leq k \leq v - 2$. For admissible contractions, we have*

$$\frac{(v-2)!}{(v-k-2)!} x(\Gamma) = \sum_{\substack{e_{i_1} \in \\ E(\Gamma)}} \frac{R_{i_1}}{L_{i_1} + R_{i_1}} \sum_{\substack{e_{i_2} \in \\ E(\overline{\Gamma}_{i_1})}} \frac{R_{i_2}}{L_{i_2} + R_{i_2}} \cdots \sum_{\substack{e_{i_k} \in \\ E(\overline{\Gamma}_{i_1,\ldots,i_{k-1}})}} \frac{R_{i_k}}{L_{i_k} + R_{i_k}} x(\overline{\Gamma}_{i_1,\ldots,i_k}),$$

$$\frac{(v-2)!}{(v-k-2)!} y(\Gamma) = \sum_{\substack{e_{i_1} \in \\ E(\Gamma)}} \frac{R_{i_1}}{L_{i_1} + R_{i_1}} \sum_{\substack{e_{i_2} \in \\ E(\overline{\Gamma}_{i_1})}} \frac{R_{i_2}}{L_{i_2} + R_{i_2}} \cdots \sum_{\substack{e_{i_k} \in \\ E(\overline{\Gamma}_{i_1,\ldots,i_{k-1}})}} \frac{R_{i_k}}{L_{i_k} + R_{i_k}} y(\overline{\Gamma}_{i_1,\ldots,i_k}).$$

Proof. We have $\frac{R_{i_j}}{L_{i_j}+R_{i_j}} = 0$ for an edge e_{i_j} that is a self loop. Thus, contraction of self loops does not contribute to sums in contraction identities. Applying Theorem 4.9 inductively gives the result. ■

Note that Theorem 4.11 generalizes the similar results in [6] to any metrized graph.

Next, we take the advantage of the contraction formula to derive Theorem 4.12 which is our second main result. It describes how the Kirchhoff index changes under successive edge contractions.

Theorem 4.12. *Let Γ be a metrized graph with $v \geq 5$ vertices, and let k be an integer with $1 \leq k \leq v-4$. For admissible contractions, we have*

$$Kf(\Gamma) = \frac{(v-4-k)!}{(v-4)!} \sum_{\substack{e_{i_1} \in \\ E(\Gamma)}} \frac{R_{i_1}}{L_{i_1}+R_{i_1}} \sum_{\substack{e_{i_2} \in \\ E(\overline{\Gamma}_{i_1})}} \frac{R_{i_2}}{L_{i_2}+R_{i_2}} \cdots \sum_{\substack{e_{i_k} \in \\ E(\overline{\Gamma}_{i_1,\dots,i_{k-1}})}} \frac{R_{i_k}}{L_{i_k}+R_{i_k}} Kf(\overline{\Gamma}_{i_1,\dots,i_k})$$
$$- \frac{\big(v^2-(k+2)v+k-1\big)k}{(v-k-2)(v-k-3)} y(\Gamma).$$

In particular, if $k = v-4$, we have

$$Kf(\Gamma) = \frac{1}{(v-4)!} \sum_{\substack{e_{i_1} \in \\ E(\Gamma)}} \frac{R_{i_1}}{L_{i_1}+R_{i_1}} \cdots \sum_{\substack{e_{i_{v-4}} \in \\ E(\overline{\Gamma}_{i_1,\dots,i_{v-5}})}} \frac{R_{i_{v-4}}}{L_{i_{v-4}}+R_{i_{v-4}}} Kf(\overline{\Gamma}_{i_1,\dots,i_{v-4}})$$
$$- \frac{(3v-5)(v-4)}{2} y(\Gamma).$$

Proof. The proof follows by successive application of Theorem 4.5 for each $Kf(\overline{\Gamma}_{i_1,\dots,i_k})$ and Theorem 4.9 for each $y(\overline{\Gamma}_{i_1,\dots,i_k})$. One should be careful about determining the coefficient of $y(\Gamma)$ after each contraction step. Note that we can compute the coefficient of $y(\Gamma)$ at the k-th contraction step with the help of the following identity:

$$\frac{v}{v-4} + \sum_{i=1}^{k-1} \frac{v-i}{v-4-i} \prod_{j=1}^{i} \frac{v-1-j}{v-3-j} = \frac{\big(v^2-(k+2)v+k-1\big)k}{(v-k-2)(v-k-3)} . \blacksquare$$

Note that $\overline{\Gamma}_{i_1,\dots,i_{v-4}}$ has 4 vertices. Therefore, it is important to know the relation between $Kf(\Gamma)$ and $y(\Gamma)$ when Γ has 4 edges to derive further conclusions from Theorem 4.12. Although the exact relation as in Corollary 4.10 is not possible in general, we can have upper and lower bounds of $Kf(\Gamma)$ in terms of $y(\Gamma)$. This is what we show below. First, we recall some facts.

Let the set of vertices for an admissible contraction $\overline{\Gamma}_{i_1,i_2,\dots,i_{v-2}}$ of Γ be $\{p', q'\}$. Suppose that m vertices of Γ are contracted into p' and that the remaining k vertices are contracted into q'. Then both m and k are positive integers with $m+k=v$, where v is the number of vertices in Γ.

Next, we state a corollary to Theorem 4.11. It generalizes the relevant result from [6] to any metrized graph possibly with bridges.

Corollary 4.13. *Let Γ be a metrized graph with v vertices. For admissible contractions $\overline{\Gamma}_{i_1,\dots,i_{v-2}}$, we have*

$$(v-2)!\,y(\Gamma) = \sum_{\substack{e_{i_1} \in \\ E(\Gamma)}} \frac{R_{i_1}}{L_{i_1}+R_{i_1}} \sum_{\substack{e_{i_2} \in \\ E(\overline{\Gamma}_{i_1})}} \frac{R_{i_2}}{L_{i_2}+R_{i_2}} \cdots \sum_{\substack{e_{i_{v-2}} \in \\ E(\overline{\Gamma}_{i_1,\dots,i_{v-3}})}} \frac{R_{i_{v-2}}}{L_{i_{v-2}}+R_{i_{v-2}}} r_{\overline{\Gamma}_{i_1,\dots,i_{v-2}}}(p',q').$$

Proof. First we note that $y(\overline{\Gamma}_{i_1,\dots,i_{v-2}}) = r_{\overline{\Gamma}_{i_1,\dots,i_{v-2}}}(p',q')$ by the proof of [6, Proposition 5.8].

Then the result follows from Theorem 4.11 with $k = v-2$. ■

Since we obtained the contraction formula in Theorem 4.7 for any metrized graph not necessarily bridgeless, we can extend the contraction formula for the Kirchhoff index given in [7, Lemma 5.2] to all metrized graphs:

Lemma 4.14. *Let Γ be a metrized graph with v vertices, and let m and k be defined as above. For any admissible contraction $\overline{\Gamma}_{i_1,i_2,\dots,i_{v-2}}$, we have*

$$Kf(\Gamma) = \frac{1}{(v-2)!}\sum_{\substack{e_{i_1}\in\\ E(\Gamma)}}\frac{R_{i_1}}{L_{i_1}+R_{i_1}}\cdots\sum_{\substack{e_{i_{v-2}}\in\\ E(\overline{\Gamma}_{i_1,\dots,i_{v-3}})}}\frac{R_{i_{v-2}}}{L_{i_{v-2}}+R_{i_{v-2}}}m\cdot k\cdot r_{\overline{\Gamma}_{i_1,\dots,i_{v-2}}}(p',q').$$

The following upper bound was given in [7, Equation 21] for regular graphs that are bridgeless. Now, we have it without any restriction on Γ:

Corollary 4.15. *For any metrized graph Γ with v vertices, we have*

$$Kf(\Gamma) \leq \frac{v^2}{4}y(\Gamma).$$

Proof. When $m+k=v$ for any two positive integers m and k, the maximum of $m\cdot k$ is at most $\frac{v^2}{4}$. Then the proof follows from Lemma 4.14 and Corollary 4.13. ■

Lemma 4.16. *Let Γ be a metrized graph with v vertices. Then we have*

$$3y(\Gamma) \leq Kf(\Gamma) \leq 4y(\Gamma) \qquad \text{if } v=4,$$
$$4y(\Gamma) \leq Kf(\Gamma) \leq 6y(\Gamma) \qquad \text{if } v=5.$$

Proof. We apply the contraction formula given in Lemma 4.14 to Γ. Since $m+k=v$ and both m and k are positive integers, if $v=4$, then we either have $m\cdot k=3$ or $m\cdot k=4$, and if $v=5$, then we either have $m\cdot k=4$ or $m\cdot k=6$. Thus, the inequalities in the lemma follows from Corollary 4.13. ■

Now, using Lemma 4.16 for $\overline{\Gamma}_{i_1,\dots,i_{v-4}}$, Theorem 4.12 and Theorem 4.11 with $k=v-4$, we derive the following proposition if $v\geq 4$. Whenever $v=2$ or $v=3$, the upper and lower bounds in this proposition become equal, so the proposition in this case is nothing but Corollary 4.10.

Proposition 4.17. *For any metrized graph with v vertices, we have*
$$(v-1)y(\Gamma) \leq Kf(\Gamma) \leq \frac{v^2-3v+4}{2}y(\Gamma).$$

We note that when $v \geq 5$ Corollary 4.15 gives better upper bounds than Proposition 4.17.

Next, we give an example to illustrate how the contraction formula in Theorem 4.12 can be used.

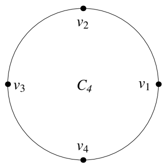

Figure 4: Circle graph with 4 vertices

Example I: Let C_v be the circle graph with v vertices and v edges. Figure 4 illustrates C_4. Suppose each edge length of the metrized graph $\Gamma = C_v$ is equal to 1. Then $\ell(C_v) = v$, and we have $Kf(C_4) = 5$ by direct computation. Moreover, $\tau(\Gamma) = \frac{1}{12}\ell(C_v)$ by [5, Corollary 2.17], $\tau(\Gamma) = \frac{1}{12}\ell(C_v) - \frac{x(\Gamma)-y(\Gamma)}{6}$ by [6, Equation 20], $x(\Gamma)+y(\Gamma) = \frac{v-1}{v}\ell(C_v)$ by [7, Lemma 6.3]. Thus, $x(\Gamma) = y(\Gamma) = \frac{v-1}{2}$.

Since $\overline{\Gamma}_{i_1,\dots,i_{v-4}} = C_4$ for every admissible contraction of Γ in this case, applying Theorem 4.12 with $k = v-4$ gives $Kf(C_v) = \frac{v(v^2-1)}{12}$. This agrees with the result obtained in [17, Equation (5)].

Next, we express the contraction formula for the Kirchhoff index in Theorem 4.12 in terms of the traces of the pseudo inverses of related discrete Laplacian matrices.

Let β be the metrized graph obtained from Γ as follows: First, we delete any possible self loops in Γ. Then we replace multiple edges with end points p_i and q_i by one edge with the same end points and having length equal to the effective resistance between the end points of those multiple edges. For example, multiple edges with lengths a and b is replaced by an edge with length $\frac{ab}{a+b}$. Suppose $\beta_{i_1,i_2,\dots,i_k}$ is the metrized graph obtained from $\overline{\Gamma}_{i_1,\dots,i_k}$ by following similar procedure. Then we have the following observations:

We have $V(\beta) = V(\Gamma) = v$ and $V(\beta_{i_1,i_2,\dots,i_k}) = V(\overline{\Gamma}_{i_1,\dots,i_k}) = v-k$. For any p, q in $V(\beta)$, $r_\beta(p,q) = r_\Gamma(p,q)$. Similarly, the resistance between any two vertices in $\beta_{i_1,i_2,\dots,i_k}$ is equal to the resistance between those vertices in $\overline{\Gamma}_{i_1,\dots,i_k}$. Therefore, we have $Kf(\beta) = Kf(\Gamma)$

and $Kf(\beta_{i_1,i_2,\dots,i_k}) = Kf(\overline{\Gamma}_{i_1,\dots,i_k})$. Next, we recall the following fact ([22] and [11])

$$Kf(\beta) = v \cdot \mathrm{tr}(\mathrm{L}^+), \quad \text{where } \mathrm{L}^+ \text{ is the pseudo inverse of the discrete Laplacian of } \beta.$$

Let $\mathrm{L}^+_{\mathrm{i_1,i_2,\dots,i_k}}$ be the pseudo inverse of the discrete Laplacian matrix of $\beta_{i_1,i_2,\dots,i_k}$. Now, we can rewrite Theorem 4.12 as follows:

Theorem 4.18. *Let Γ be a metrized graph with $v \geq 5$ vertices, and let k be an integer with $1 \leq k \leq v-4$. Using the notations above, we have the following equality for admissible contractions:*

$$tr(\mathrm{L}^+) = \frac{(v-4-k)!(v-k)}{(v-4)!v} \sum_{\substack{e_{i_1}\in \\ E(\Gamma)}} \frac{R_{i_1}}{L_{i_1}+R_{i_1}} \cdots \sum_{\substack{e_{i_k}\in \\ E(\overline{\Gamma}_{i_1,\dots,i_{k-1}})}} \frac{R_{i_k}}{L_{i_k}+R_{i_k}} tr(\mathrm{L}^+_{\mathrm{i_1,i_2,\dots,i_k}})$$
$$- \frac{\big(v^2-(k+2)v+k-1\big)k}{(v-k-2)(v-k-3)v} y(\Gamma).$$

In particular, if $k = v-4$, we have

$$tr(\mathrm{L}^+) = \frac{4}{(v-4)!v} \sum_{\substack{e_{i_1}\in \\ E(\Gamma)}} \frac{R_{i_1}}{L_{i_1}+R_{i_1}} \cdots \sum_{\substack{e_{i_{v-4}}\in \\ E(\overline{\Gamma}_{i_1,\dots,i_{v-5}})}} \frac{R_{i_{v-4}}}{L_{i_{v-4}}+R_{i_{v-4}}} tr(\mathrm{L}^+_{\mathrm{i_1,i_2,\dots,i_{v-4}}})$$
$$- \frac{(3v-5)(v-4)}{2v} y(\Gamma).$$

Note that in Theorem 4.12, we expressed $Kf(\Gamma)$ in terms of the Kirchhoff indices of the metrized graphs $\overline{\Gamma}_{i_1,\dots,i_{v-4}}$ having 4 vertices and the quantity $y(\Gamma)$. In fact, we can apply Proposition 4.6 and the contraction formula of $y(\Gamma)$ to make one further contraction to express $Kf(\Gamma)$ in terms of the resistance values between the vertices of $\overline{\Gamma}_{i_1,\dots,i_{v-3}}$ having 3 vertices.

Theorem 4.19. *Let Γ be a metrized graph with $v \geq 4$ vertices. For admissible contractions, we have*

$$Kf(\Gamma) = \frac{1}{(v-4)!} \sum_{\substack{e_{i_1}\in \\ E(\Gamma)}} \frac{R_{i_1}}{L_{i_1}+R_{i_1}} \cdots \sum_{\substack{e_{i_{v-3}}\in \\ E(\overline{\Gamma}_{i_1,\dots,i_{v-4}})}} \frac{R_{i_{v-3}}}{L_{i_{v-3}}+R_{i_{v-3}}} \Big[A\big(r'(p,\overline{p}_{i_{v-3}}) + r'(q,\overline{p}_{i_{v-3}})\big)$$
$$- B \cdot r'(p,q)\Big],$$

where $A = \frac{v^2-3v+4}{4(v-2)(v-3)}$, $B = \frac{v^2-7v+8}{4(v-2)(v-3)}$, and $r'(x,y)$ is the resistance function in $\overline{\Gamma}_{i_1,\dots,i_{v-3}}$ having the vertex set $\{p,q,\overline{p}_{i_{v-3}}\}$. Here the end points of the edge $e_{i_{v-3}}$ are contracted into the vertex $\overline{p}_{i_{v-3}}$.

Proof. It follows from Theorem 4.11 that

$$y(\Gamma) = \frac{2}{(v-2)!} \sum_{\substack{e_{i_1} \in \\ E(\Gamma)}} \frac{R_{i_1}}{L_{i_1} + R_{i_1}} \sum_{\substack{e_{i_2} \in \\ E(\overline{\Gamma}_{i_1})}} \frac{R_{i_2}}{L_{i_2} + R_{i_2}} \cdots \sum_{\substack{e_{i_{v-4}} \in \\ E(\overline{\Gamma}_{i_1,\dots,i_{v-5}})}} \frac{R_{i_{v-4}}}{L_{i_{v-4}} + R_{i_{v-4}}} y(\overline{\Gamma}_{i_1,\dots,i_{v-4}}).$$

Using this equality in the contraction formula given in Theorem 4.12 we derive

$$Kf(\Gamma) = \frac{1}{(v-4)!} \sum_{\substack{e_{i_1} \in \\ E(\Gamma)}} \frac{R_{i_1}}{L_{i_1} + R_{i_1}} \cdots \sum_{\substack{e_{i_{v-4}} \in \\ E(\overline{\Gamma}_{i_1,\dots,i_{v-5}})}} \frac{R_{i_{v-4}}}{L_{i_{v-4}} + R_{i_{v-4}}} \Big[Kf(\overline{\Gamma}_{i_1,\dots,i_{v-4}}) - \frac{(3v-5)(v-4)}{(v-2)(v-3)} y(\overline{\Gamma}_{i_1,\dots,i_{v-4}}) \Big].$$

We use Proposition 4.6 to obtain

$$2Kf(\overline{\Gamma}_{i_1,\dots,i_{v-4}}) = 4y(\overline{\Gamma}_{i_1,\dots,i_{v-4}}) + \sum_{\substack{e_{i_{v-3}} \in \\ E(\overline{\Gamma}_{i_1,\dots,i_{v-4}})}} \frac{R_{i_{v-3}}}{L_{i_{v-3}} + R_{i_{v-3}}} \sum_{\substack{s \in \\ V(\overline{\Gamma}_{i_1,\dots,i_{v-3}})}} r'(s, \overline{p}_{i_{v-3}}).$$

Now, we obtain the following equality by using Theorem 4.5:

$$y(\overline{\Gamma}_{i_1,\dots,i_{v-4}}) = \frac{1}{4} \sum_{\substack{e_{i_{v-3}} \in \\ E(\overline{\Gamma}_{i_1,\dots,i_{v-4}})}} \frac{R_{i_{v-3}}}{L_{i_{v-3}} + R_{i_{v-3}}} Kf(\overline{\Gamma}_{i_1,\dots,i_{v-3}}).$$

If we use the last two equality in the contraction formula above for $Kf(\Gamma)$, we obtain

$$Kf(\Gamma) = \frac{1}{(v-4)!} \sum_{\substack{e_{i_1} \in \\ E(\Gamma)}} \frac{R_{i_1}}{L_{i_1} + R_{i_1}} \cdots \sum_{\substack{e_{i_{v-3}} \in \\ E(\overline{\Gamma}_{i_1,\dots,i_{v-4}})}} \frac{R_{i_{v-3}}}{L_{i_{v-3}} + R_{i_{v-3}}} \Big[\frac{1}{2} \sum_{\substack{s \in \\ V(\overline{\Gamma}_{i_1,\dots,i_{v-3}})}} r'(s, \overline{p}_{i_{v-3}}) - \frac{v^2 - 7v + 8}{4(v-2)(v-3)} Kf(\overline{\Gamma}_{i_1,\dots,i_{v-3}}) \Big].$$

Hence, the result follows by noting that

$$\sum_{\substack{s \in \\ V(\overline{\Gamma}_{i_1,\dots,i_{v-3}})}} r'(s, \overline{p}_{i_{v-3}}) = r'(p, \overline{p}_{i_{v-3}}) + r'(q, \overline{p}_{i_{v-3}}),$$

$$Kf(\overline{\Gamma}_{i_1,\dots,i_{v-3}}) = r'(p, \overline{p}_{i_{v-3}}) + r'(q, \overline{p}_{i_{v-3}}) + r'(p, q),$$

where p, q and $\overline{p}_{i_{v-3}}$ are the three vertices of $\overline{\Gamma}_{i_1,\dots,i_{v-3}}$. ■

As we have seen in Theorem 4.19, there is a need to know the resistance values between the vertices of a metrized graph with 3 vertices.

Suppose Γ_1 and Γ_2 are metrized graphs having vertex sets $\{p, q, s\}$, edge lengths 1, and no self loops. In Γ_1, we have $k \geq 1$ edges with end points p and q, and $u \geq 1$ edges

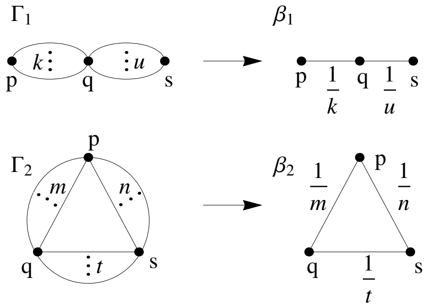

Figure 5: Metrized graphs Γ_1 and Γ_2 having circuit reductions β_1 and β_2.

connecting the vertices q and s. In Γ_2, there are $m \geq 1$, $n \geq 1$ and $t \geq 1$ edges having the end points $\{q, p\}$, $\{p, s\}$ and $\{s, q\}$, respectively. By replacing any multiple edges by an edge with length equal to the effective resistance between their end points we obtain the graphs β_1 and β_2. Figure 5 illustrates these graphs. Then it is easy to compute the resistance values between the vertices of these graphs as follows:

$$r_{\Gamma_1}(p,q) = \frac{1}{k}, \quad r_{\Gamma_1}(p,s) = \frac{1}{k} + \frac{1}{u}, \quad r_{\Gamma_1}(q,s) = \frac{1}{u}$$
$$r_{\Gamma_2}(p,q) = \frac{n+t}{mn+mt+nt}, \quad r_{\Gamma_2}(p,s) = \frac{m+t}{mn+mt+nt}, \quad r_{\Gamma_2}(s,q) = \frac{m+n}{mn+mt+nt}. \tag{15}$$

Therefore, if Γ is a metrized graph with each edge length 1, the term

$$A\big(r'(p, \overline{p}_{i_{v-3}}) + r'(q, \overline{p}_{i_{v-3}})\big) - B \cdot r'(p,q)$$

in Theorem 4.19 is equal to one of the following values:

$$\begin{array}{ll}
(A-B)\frac{1}{u} + 2A\frac{1}{k}, & \text{if } \overline{\Gamma}_{i_1,\dots,i_{v-3}} = \Gamma_1 \text{ and } \overline{p}_{i_{v-3}} = p. \\
(A-B)(\frac{1}{k} + \frac{1}{u}), & \text{if } \overline{\Gamma}_{i_1,\dots,i_{v-3}} = \Gamma_1 \text{ and } \overline{p}_{i_{v-3}} = q. \\
(A-B)\frac{1}{k} + 2A\frac{1}{u}, & \text{if } \overline{\Gamma}_{i_1,\dots,i_{v-3}} = \Gamma_1 \text{ and } \overline{p}_{i_{v-3}} = s. \\
(A-B)\frac{m+n}{mn+mt+nt} + 2A\frac{t}{mn+mt+nt}, & \text{if } \overline{\Gamma}_{i_1,\dots,i_{v-3}} = \Gamma_2 \text{ and } \overline{p}_{i_{v-3}} = p. \\
(A-B)\frac{m+t}{mn+mt+nt} + 2A\frac{n}{mn+mt+nt}, & \text{if } \overline{\Gamma}_{i_1,\dots,i_{v-3}} = \Gamma_2 \text{ and } \overline{p}_{i_{v-3}} = q. \\
(A-B)\frac{n+t}{mn+mt+nt} + 2A\frac{m}{mn+mt+nt}, & \text{if } \overline{\Gamma}_{i_1,\dots,i_{v-3}} = \Gamma_2 \text{ and } \overline{p}_{i_{v-3}} = s.
\end{array}$$

Lower and upper bounds to these values over all admissible contractions lead to lower and upper bounds to the Kirchhoff index. For example, if Λ is the edge connectivity of

Γ, one can show that $(4A-2B)\frac{1}{\Lambda}$ is an upper bound to these values over all admissible contractions. Because we have $\Lambda \leq \min\{u, k\}$ and $\Lambda \leq \{m+n, m+t, n+t\}$. Then this upper bound and Theorem 4.19 lead to the upper bound $Kf(\Gamma) \leq \frac{v(v^2-1)}{4\Lambda}$ for any metrized graph Γ. We show that better upper bounds can be given in the next section.

5 The Kirchhoff Index and Edge Densities

In the last section, we obtained a contraction formula in Lemma 4.14 that relates the Kirchhoff index of a metrized graph Γ and Kirchhoff indices of an admissible contractions $\overline{\Gamma}_{i_1,\dots,i_{v-2}}$. Now, we give another interpretation of this formula by relating admissible contractions of Γ to admissible partitions of $V(\Gamma)$.

For an admissible contraction $\overline{\Gamma}_{i_1,i_2,\dots,i_{v-2}}$ having the set of vertices $\{p', q'\}$, suppose that $1 \leq m$ and $1 \leq k$ vertices of Γ are contracted into p' and q', respectively. If the number of edges connecting p' and q' is n', we know that $\Lambda = \min\{n'\}$, where the minimum is taken over all admissible contractions and Λ is the edge connectivity of Γ (see [6, Lemma 6.2]). Moreover, if each edge of Γ has length 1, then $r_{\overline{\Gamma}_{i_1,\dots,i_{v-2}}}(p', q') = \frac{1}{n'}$. If Γ has e number of edges, we have $n' \leq e - v + 2$ as we contracted $v-2$ edges to obtain $\overline{\Gamma}_{i_1,\dots,i_{v-2}}$.

Suppose the set of vertices contracted into p' and q' are V_1 and V_2, respectively. Note that $\{V_1, V_2\}$ is an admissible partition of $V(\Gamma)$ and that $|E(V_1, V_2)| = n'$, $|V_1| = m$ and $|V_2| = k$. Therefore, we have the following equality

$$m \cdot k \cdot r_{\overline{\Gamma}_{i_1,\dots,i_{v-2}}}(p', q') = \frac{1}{d(V_1, V_2)}. \tag{16}$$

Using the formula in Lemma 4.14, Equation (16) and the fact that

$$(v-1)! = \sum_{\substack{e_{i_1}\in \\ E(\Gamma)}} \frac{R_{i_1}}{L_{i_1}+R_{i_1}} \sum_{\substack{e_{i_2}\in \\ E(\overline{\Gamma}_{i_1})}} \frac{R_{i_2}}{L_{i_2}+R_{i_2}} \cdots \sum_{\substack{e_{i_{v-2}}\in \\ E(\overline{\Gamma}_{i_1,\dots,i_{v-3}})}} \frac{R_{i_{v-2}}}{L_{i_{v-2}}+R_{i_{v-2}}},$$

we obtain the following result:

Theorem 5.1. *Let Γ be a metrized graph with set of vertices $V(\Gamma)$, and let each edge of Γ have length 1. Then we have*

$$\frac{v-1}{d_{\max}} \leq Kf(\Gamma) \leq \frac{v-1}{d_{min}}.$$

Since $1 \leq m$, $1 \leq k$ and $m+k = v$, we have $v-1 \leq m \cdot k \leq \frac{v^2}{4}$. Using these inequalities, Equation (16) and the fact that $\Lambda \leq n' \leq e-v+2$, we obtain the following inequalities:

$$\frac{4\Lambda}{v^2} \leq d_{\min}, \quad \text{and} \quad d_{\max} \leq \frac{e-v+2}{v-1}. \tag{17}$$

Thus, the following corollary follows from these inequalities and Theorem 5.1.

Corollary 5.2. *Let Γ be a metrized graph with e edges and $v \geq 2$ vertices, and let each edge of Γ have length 1. Then we have*

$$\frac{(v-1)^2}{e-v+2} \leq Kf(\Gamma) \leq \frac{v^2(v-1)}{4\Lambda},$$

where Λ is the edge connectivity of Γ.

Note that if the metrized graph with vertex set $V(\Gamma)$ is a simple graph, then $d_{\max} \leq 1$, in which case we have $(v-1) \leq Kf(\Gamma)$.

6 Trees, When the Kirchhoff Index is the Wiener Index

In this section, we restrict ourselves to tree metrized graphs. A tree graph is a connected graph with no cycle. That is, each edge in a tree graph is a bridge. We rewrite many of the results from §4 for tree metrized graphs. In this way, when the graph is a tree, we derive new formulas as well as previously known formulas for the Wiener index with new proofs.

Let $d(p,q)$ denote the distance between the vertices p and q in $V(\Gamma)$. Then the Wiener index of Γ is defined as follows (see [9, Page 211] and the references therein):

$$W(\Gamma) := \frac{1}{2} \sum_{p,\, q \in V(\Gamma)} d(p,q).$$

This formula was first given in [13] but the concept of the Wiener number was introduced in [14].

When Γ is a tree, $d(p,q) = r(p,q)$ for each vertices p and q, where $r(x,y)$ is the resistance function on Γ. Therefore,

$$W(\Gamma) = Kf(\Gamma) \quad \text{if } \Gamma \text{ is a tree.} \tag{18}$$

When Γ is a tree, Lemma 4.3 can be restated as follows

Lemma 6.1. *Let* Γ *be a metrized graph that is a tree with* υ *vertices. For any* $p \in V(\Gamma)$*, we have*

$$\ell(\Gamma) = \sum_{q \in V(\Gamma)} (2 - \upsilon(q)) r(p, q).$$

In particular, if each edge length is equal to 1*, we have*

$$\upsilon - 1 = \sum_{q \in V(\Gamma)} (2 - \upsilon(q)) r(p, q).$$

Proof. Each edge is a bridge in Γ as it is a tree. Thus, we have $(R_{a_i,p} - R_{b_i,p})^2 = R_i^2$ for each edge in Γ, and so $\frac{L_i(R_{a_i,p}-R_{b_i,p})^2}{(L_i+R_i)^2} = \frac{L_i R_i^2}{(L_i+R_i)^2}$. We have $\frac{L_i R_i^2}{(L_i+R_i)^2} \longrightarrow L_i$ and $\frac{L_i}{L_i+R_i} \longrightarrow 0$ as $R_i \longrightarrow \infty$. Therefore, the first equality in the lemma follows from the first equality given in Lemma 4.3. When $L_i = 1$ for every $e_i \in E(\Gamma)$, the second equality in the lemma is obtained by using the fact that $\ell(\Gamma) = e = \upsilon - 1$, where e is the number of edges of Γ. ∎

Theorem 6.2. *Let* Γ *be a metrized graph that is a tree with* υ *vertices. Then we have*

$$W(\Gamma) = \frac{1}{4}\Big[\upsilon \cdot \ell(\Gamma) + \sum_{p,\, q \in V(\Gamma)} \upsilon(q) r(p, q)\Big].$$

In particular, if each edge length is equal to 1*, we have*

$$W(\Gamma) = \frac{1}{4}\Big[\upsilon(\upsilon - 1) + \sum_{p,\, q \in V(\Gamma)} \upsilon(q) r(p, q)\Big].$$

Proof. We take the summation of the equalities given in Lemma 6.1 over all vertices $p \in V(\Gamma)$. Then we obtain the result by using the definition of $W(\Gamma)$. ∎

Note that the result given in Theorem 6.2 was known in the literature for trees with equal edge lengths (see [9, Page 217] and the references therein).

Now, we can state our first main result for trees:

Theorem 6.3. *Let* Γ *be a metrized graph that is a tree with* υ *vertices. Then we have*

$$W(\Gamma) = \frac{2\upsilon - 1}{4}\ell(\Gamma) + \frac{1}{8}\sum_{p,\, q \in V(\Gamma)} \upsilon(p)\upsilon(q) r(p, q).$$

In particular, if each edge length is equal to 1*, we have*

$$W(\Gamma) = \frac{(2\upsilon - 1)(\upsilon - 1)}{4} + \frac{1}{8}\sum_{p,\, q \in V(\Gamma)} \upsilon(p)\upsilon(q) r(p, q).$$

Proof. We first multiply both sides of the first equality given in Lemma 6.1 by $2 - \upsilon(p)$. Then we take the summation of both sides over all vertices $p \in V(\Gamma)$. This gives

$$\ell(\Gamma) \sum_{p \in V(\Gamma)} (2 - \upsilon(p)) = \sum_{p,\, q \in V(\Gamma)} (2 - \upsilon(p))(2 - \upsilon(q)) r(p, q).$$

Since $\sum_{p \in V(\Gamma)} (2 - \upsilon(p)) = 2v - 2e = 2$, we have

$$\begin{aligned} 2\ell(\Gamma) &= \sum_{p,\, q \in V(\Gamma)} (2 - \upsilon(p))(2 - \upsilon(q)) r(p, q). \quad \text{Using the definition of } W(\Gamma) \text{ gives} \\ &= 8W(\Gamma) + \sum_{p,\, q \in V(\Gamma)} \upsilon(p)\upsilon(q) r(p, q) - 4 \sum_{p,\, q \in V(\Gamma)} \upsilon(q) r(p, q), \\ &= -8W(\Gamma) + 4v \cdot \ell(\Gamma) + \sum_{p,\, q \in V(\Gamma)} \upsilon(p)\upsilon(q) r(p, q), \quad \text{by Theorem 6.2.} \end{aligned}$$

This gives the first equality. The second equality follows from the first one by using the fact that $\ell(\Gamma) = v - 1$ when each edge length is equal to 1. ■

A discussion similar to the proof of Lemma 6.1 gives

$$x(\Gamma) = 0 \ \text{ and } \ y(\Gamma) = \ell(\Gamma) \text{ if } \Gamma \text{ is a tree.} \tag{19}$$

Next, we restate Theorem 4.12 for a tree:

Theorem 6.4. *Let metrized graph* Γ *be a tree with* $v \geq 5$ *vertices. and let* k *be an integer with* $1 \leq k \leq v - 4$. *For admissible contractions, we have*

$$W(\Gamma) = \frac{(v-4-k)!}{(v-4)!} \sum_{\substack{e_{i_1} \in \\ E(\Gamma)}} \cdots \sum_{\substack{e_{i_k} \in \\ E(\overline{\Gamma}_{i_1,\dots,i_{k-1}})}} W(\overline{\Gamma}_{i_1,\dots,i_k}) - \frac{\big(v^2 - (k+2)v + k - 1\big)k}{(v-k-2)(v-k-3)} \ell(\Gamma).$$

In particular, if $k = v - 4$, *we have*

$$W(\Gamma) = \frac{1}{(v-4)!} \sum_{\substack{e_{i_1} \in \\ E(\Gamma)}} \sum_{\substack{e_{i_2} \in \\ E(\overline{\Gamma}_{i_1})}} \cdots \sum_{\substack{e_{i_{v-4}} \in \\ E(\overline{\Gamma}_{i_1,\dots,i_{v-5}})}} W(\overline{\Gamma}_{i_1,\dots,i_{v-4}}) - \frac{(3v-5)(v-4)}{2} \ell(\Gamma).$$

Proof. Since each edge is a bridge, we have $\frac{R_i}{L_i + R_i} \longrightarrow 1$ for each edge e_i in Γ. Then the result follows from Theorem 4.12, Equation (19) and Equation (18). ■

To derive further results about $W(\Gamma)$ by using Theorem 6.4, we need to understand the Wiener index of $\overline{\Gamma}_{i_1,\dots,i_{v-4}}$ which is a tree with 4 vertices. Thus, we consider Lemma 6.5 below.

Let S_n and P_n be star and path metrized graphs on n vertices, respectively. Figure 6 illustrates S_4 and P_4.

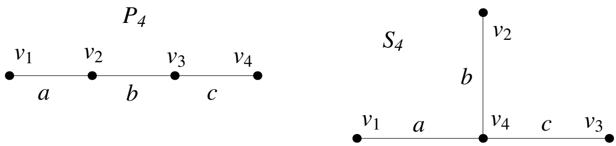

Figure 6: Path and star graphs with 4 vertices

Lemma 6.5. *Suppose metrized graph Γ is a tree with 4 vertices. Then Γ is either S_4 or P_4. Moreover, $W(P_4) = 3(a+b+c)+b$ and $W(S_4) = 3(a+b+c)$, where edge lengths are as in Figure 6.*

Proof. A direct computation gives the result. ∎

Now, we can state our second main result for trees:

Theorem 6.6. *Let metrized graph Γ be a tree with v vertices. Suppose each edge length of Γ is 1. Then we have*

$$W(\Gamma) = (v-1)^2 + \sum_{\substack{\{e_{i_1}, e_{i_2}, \cdots, e_{i_{v-4}}\} \subset E(\Gamma) \\ \overline{\Gamma}_{i_1,\dots,i_{v-4}} = P_4}} 1,$$

$$= (v-1)^2 + \sum_{\substack{\{e_{i_1}, e_{i_2}, e_{i_3}\} \subset E(\Gamma) \\ e_{i_1}, e_{i_2}, e_{i_3} \in P \\ P \text{ is a path in } \Gamma}} 1.$$

The last summation is taken over all subsets $\{e_{i_1}, e_{i_2}, e_{i_3}\}$ of $E(\Gamma)$ such that the edges e_{i_1}, e_{i_2} and e_{i_3} are parts of a path in Γ.

Proof. Applying Lemma 6.5 for this case, we obtain $W(\overline{\Gamma}_{i_1,\dots,i_{v-4}}) = 10$ if $\overline{\Gamma}_{i_1,\dots,i_{v-4}} = P_4$, and $W(\overline{\Gamma}_{i_1,\dots,i_{v-4}}) = 9$ if $\overline{\Gamma}_{i_1,\dots,i_{v-4}} = S_4$.

We note that

$$\frac{1}{(v-4)!} \sum_{\substack{e_{i_1} \in \\ E(\Gamma)}} \sum_{\substack{e_{i_2} \in \\ E(\overline{\Gamma}_{i_1})}} \cdots \sum_{\substack{e_{i_{v-4}} \in \\ E(\overline{\Gamma}_{i_1,\dots,i_{v-5}})}} 1 = \frac{(v-1)(v-2)(v-3)}{6}.$$

Then we use Theorem 6.4 with $\ell(\Gamma) = (v-1)$ to obtain

$$W(\Gamma) = (v-1)^2 + \frac{1}{(v-4)!} \sum_{\substack{e_{i_1}, e_{i_2}, \cdots, e_{i_{v-4}} \in E(\Gamma) \\ \overline{\Gamma}_{i_1,\dots,i_{v-4}} = P_4}} 1 = (v-1)^2 + \sum_{\substack{\{e_{i_1}, e_{i_2}, \cdots, e_{i_{v-4}}\} \subset E(\Gamma) \\ \overline{\Gamma}_{i_1,\dots,i_{v-4}} = P_4}} 1.$$

We have the second equality above, because the number of permutations of $v-4$ edges $e_{i_1}, e_{i_2}, \cdots, e_{i_{v-4}}$ is $(v-4)!$. This gives the first equality in the theorem.

The second equality in the theorem follows from the first one. ■

Note that Theorem 6.6 in a sense gives information about how far a graph is away from being a star graph.

As a corollary to Theorem 6.6, we obtain the following well-known result:

Corollary 6.7. *For any metrized graph Γ with v vertices, we have*

$$(v-1)^2 = W(S_v) \leq W(\Gamma) \leq W(P_v) = \frac{v(v^2-1)}{6}.$$

Proof. No path in S_v can contain 3 edges, so $W(S_v) = (v-1)^2$ by using Theorem 6.6. Since this is the case with minimum value 0 of the summation in the formula of Theorem 6.6, we obtain $W(S_v) \leq W(\Gamma)$.

On the other hand, any 3 edges in P_v is part of a path in P_v, namely the path is P_v itself. Thus, the summation in the formula of Theorem 6.6 is $\binom{v-1}{3}$, and so $W(P_v) = (v-1)^2 + \binom{v-1}{3}$ by Theorem 6.6. We note that $\binom{v-1}{3}$ is the maximum value of the summation, so $W(\Gamma) \leq W(P_v)$. ■

We recall the following result due to Doyle and Graver [10] to compare with Theorem 6.6:

Theorem 6.8. *[9, Theorem 9] Let graph Γ be a tree with v vertices, and let $v_1, v_2, \ldots, v_{v(p)}$ be the number vertices in the connected components of the graph obtained from Γ by deleting the edges connected to a vertex p. Then*

$$W(\Gamma) = \frac{v(v^2-1)}{6} - \sum_{\substack{p \in V(\Gamma), \\ v(p) \geq 3}} \sum_{1 \leq i < j < k \leq v(p)} v_i v_j v_k.$$

Note that Theorem 6.8 somewhat explains how far a graph is away from being a path graph.

Next, we restate Lemma 4.14 for trees. For an edge e_i with end points p_i and q_i, let m_i be the number of vertices that are in the connected component of $\Gamma - e_i$ containing p_i, and let k_i be the number of vertices that are in the connected component of $\Gamma - e_i$ containing q_i. Then we have $m_i + k_i = v$.

Theorem 6.9. *Let metrized graph Γ be a tree with v vertices. Suppose each edge length of Γ is* 1*. Then we have*

$$W(\Gamma) = \sum_{e_i \in E(\Gamma)} m_i \cdot k_i.$$

Proof. Each edge e_i is a bridge, so $\frac{R_i}{L_i+R_i} \longrightarrow 1$. Moreover, $\overline{\Gamma}_{i_1,\dots,i_{v-2}}$ is the edge that is not contracted, so we have $r_{\overline{\Gamma}_{i_1,\dots,i_{v-2}}}(p', q') = 1$. Therefore, Lemma 4.14 implies

$$W(\Gamma) = \frac{1}{(v-2)!} \sum_{e_{i_1}, e_{i_2}, \cdots, e_{i_{v-2}} \in E(\Gamma)} m \cdot k,$$

where m and k are as defined before. Considering the permutations of the contracted edges, we can rewrite this as

$$W(\Gamma) = \sum_{\{e_{i_1}, e_{i_2}, \cdots, e_{i_{v-2}}\} \subset E(\Gamma)} m \cdot k = \sum_{e_i \in E(\Gamma)} m \cdot k.$$

Now, suppose $\overline{\Gamma}_{i_1,\dots,i_{v-2}} = e_i$. Then the number of vertices contracted into p_i is nothing but m_i, i.e., $m = m_i$. Similarly, the number of vertices contracted into q' is k_i. That is, $k = k_i$. This completes the proof. ■

Note that Theorem 6.9 was known previously [9, Page 218] and [14].

Example II: Let β_1 and β_2 be metrized graphs with $s+t+2$ and $s+t+3$ vertices, respectively. These are illustrated in Figure 7. Suppose $s \geq 0$, $t \geq 0$ and each edge length in β_1 and β_2 is equal to 1. By applying Theorem 6.6, we obtain

$W(\beta_1) = (s+t+1)^2 + \binom{s}{1}\binom{t}{1} = (s+t+1)^2 + s \cdot t.$

$W(\beta_2) = (s+t+2)^2 + \binom{s}{1}\binom{2}{1}\binom{t}{1} + \binom{s}{1}\binom{2}{2}\binom{t}{0} + \binom{s}{0}\binom{2}{2}\binom{t}{1} = (s+t+2)^2 + 2s \cdot t + s + t.$

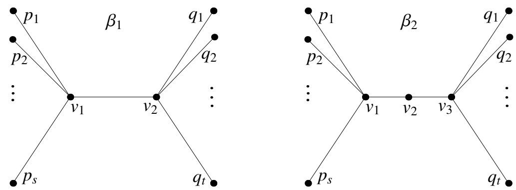

Figure 7: Tree metrized graphs β_1 and β_2.

We note that these results agree with the results given in [9, Page 234] (as $\beta_1 = D(s+t+2,s,t)$ and $\beta_2 = D(s+t+3,s,t)$, where $D(v,s,t)$ is the graph defined as in [9, Page 234]).

Example III: In this example, we work with metrized graphs β_3 and β_4 illustrated in Figure 8. β_3 and β_4 have $s+t+k+4$ and $s+t+k+m+4$ vertices, respectively. Suppose $s \geq 0$, $t \geq 0$, $k \geq 0$, $m \geq 0$ and each edge length in these graphs is equal to 1. By applying Theorem 6.6, we obtain

$$\begin{aligned} W(\beta_3) &= (s+t+k+3)^2 + \binom{s}{1}\binom{2}{1}\binom{k}{1} + \binom{s}{1}\binom{2}{2} + \binom{2}{2}\binom{k}{1} + \binom{s}{1}\binom{2}{1}\binom{t}{1} \\ &+ \binom{s}{1}\binom{2}{2} + \binom{2}{2}\binom{t}{1} + \binom{k}{1}\binom{2}{1}\binom{t}{1} + \binom{k}{1}\binom{2}{2} + \binom{2}{2}\binom{t}{1} \\ &= (s+t+k+3)^2 + 2(sk+st+kt+s+t+k). \end{aligned}$$

Now, to compute $W(\beta_4)$ we can use the computation used in obtaining $W(\beta_3)$. Namely, when we compute the number of three edges that are part of a path in β_4, we can divide the edges in two groups: The ones having an end point in $\{u_1, u_2, \cdots, u_m\}$ and the ones with no end points in this set.

$$\begin{aligned} W(\beta_4) &= (s+t+k+m+3)^2 + 2(st+(s+t)(k+1)+k) + \binom{m}{1}\left[\binom{s}{1} + \binom{k}{1} + \binom{t}{1}\right] \\ &= (s+t+k+m+3)^2 + 2(sk+st+kt) + (m+2)(s+t+k). \end{aligned}$$

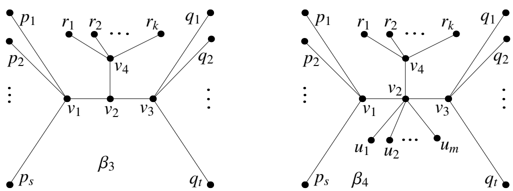

Figure 8: Tree metrized graphs β_3 and β_4.

Example IV: In this case, we work with the metrized graph β_5 illustrated in Figure 9. β_5 has $v = s+t+k+m+n+5$ vertices. Suppose $s \geq 0$, $t \geq 0$, $k \geq 0$, $m \geq 0$, $n \geq 0$ and each edge length of β_5 is equal to 1. By applying Theorem 6.6 and using the computation of $W(\beta_4)$, we obtain

$$W(\beta_5) = (v-1)^2 + 2(sk+st+kt+mn+kn+sn) + (n+2)(s+k) + (m+2)(s+k+t+1) + n(t+5).$$

The details are left as an exercise to the reader.

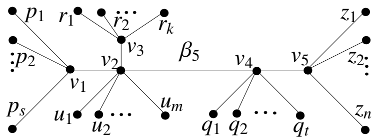

Figure 9: Tree metrized graph β_5.

Example V: In this case, we work with the metrized graph β_6 illustrated in Figure 9. β_6 has $v = s+t+k+m+n+h+6$ vertices. Suppose $s \geq 0$, $t \geq 0$, $k \geq 0$, $m \geq 0$, $n \geq 0$, $h \geq 0$ and each edge length of β_6 is equal to 1. By applying Theorem 6.6 and using the computation of $W(\beta_5)$, we obtain

$$W(\beta_6) = (v-1)^2 + 2(sk+st+kt+mn+kn+sn) + (n+4)(s+k) + n(t+6)$$
$$+ (m+2)(s+k+t+2) + h(3s+3k+2n+2m+t+6).$$

The details are left as an exercise to the reader.

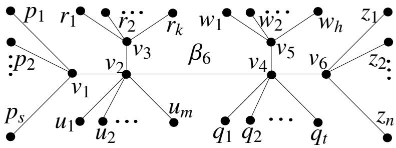

Figure 10: Tree metrized graph β_6.

Problem I: Show that the function $F : \mathbb{N}^5 \longrightarrow \mathbb{N}$ given by $F(s,t,k,m,n) = (s+t+k+m+n+4)^2 + 2(sk+st+kt+n(m+k+s)) + (n+2)(s+k) + (m+2)(s+k+t+1) + nt + 5n$ takes every integer bigger than 557, and that the only integers not assumed by F are the following 89 numbers:

$\{1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 19, 20, 21, 22, 23, 24, 25, 26, 27, 30, 33, 34, 35, 36, 37, 38, 39, 41, 43, 45, 47, 49, 51, 52, 53, 55, 56, 60, 61, 69, 73, 75, 77, 78, 79, 81, 83, 85, 87, 89, 91, 99, 101, 106, 113, 125, 129, 131, 133, 135, 141, 143, 147, 149, 157, 159, 165, 197, 199, 203, 213, 217, 219, 281, 285, 293, 301, 325, 357, 501, 509, 557\}$.

We checked by a computer program that any integer not in the list above and less than 20000 can be a value of F.

Problem II: Show that the function $G : \mathbb{N}^6 \longrightarrow \mathbb{N}$ given by $G(s,t,k,m,n,h) = (s+t+k+m+n+h+5)^2 + 2(sk+st+kt+mn+kn+sn) + (n+4)(s+k) + (m+2)(s+k+t+2) + n(t+6) + h(3s+3k+2n+2m+t+6)$ takes every integer bigger than 301, and that the only integers not assumed by G are the following 104 numbers:
$\{1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40, 41, 43, 44, 45, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 59, 60, 61, 64, 66, 69, 70, 71, 72, 73, 75, 77, 78, 79, 81, 83, 85, 87, 89, 91, 95, 98, 99, 101, 102, 106, 113, 119, 124, 127, 129, 131, 133, 135, 139, 141, 143, 147, 149, 157, 159, 165, 197, 199, 203, 213, 217, 219, 279, 293, 301\}$.

Again, we tested by a computer program that any integer not in the list above and less than 20000 can be a value of G.

The following theorem was conjectured in [16] and [12], and proved in both [21] and [20].

Theorem 6.10. *Except for exactly the following* 49 *positive integers, every positive integer is the Wiener index of some tree.*
$\{2, 3, 5, 6, 7, 8, 11, 12, 13, 14, 15, 17, 19, 21, 22, 23, 24, 26, 27, 30, 33, 34, 37, 38, 39, 41, 43, 45, 47, 51, 53, 55, 60, 61, 69, 73, 77, 78, 83, 85, 87, 89, 91, 99, 101, 106, 113, 147, 159\}$.

Note that a positive solution to any of Problem I and Problem II above will be another proof of Theorem 6.10.

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