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Steve Kirkland

*University of Manitoba*, [stephen.kirkland@umanitoba.ca](mailto:stephen.kirkland@umanitoba.ca)

Ze Zeng

*University of Manitoba*, [zengz3@icloud.com](mailto:zengz3@icloud.com)

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## KEMENY'S CONSTANT AND AN ANALOGUE OF BRAESS' PARADOX FOR TREES\*

STEVE KIRKLAND<sup>†</sup> AND ZE ZENG<sup>‡</sup>

**Abstract.** Given an irreducible stochastic matrix  $M$ , Kemeny's constant  $\mathcal{K}(M)$  measures the expected time for the corresponding Markov chain to transition from any given initial state to a randomly chosen final state. A combinatorially based expression for  $\mathcal{K}(M)$  is provided in terms of the weights of certain directed forests in a directed graph associated with  $M$ , yielding a particularly simple expression in the special case that  $M$  is the transition matrix for a random walk on a tree. An analogue of Braess' paradox is investigated, whereby inserting an edge into an undirected graph can increase the value of Kemeny's constant for the corresponding random walk. It is shown in particular that for almost all trees, there is an edge whose insertion increases the corresponding value of Kemeny's constant. Finally, it is proven that for any  $m \in \mathbb{N}$ , almost every tree  $\mathcal{T}$  has the property that there are at least  $m$  trees, none of which are isomorphic to  $\mathcal{T}$ , such that the values of Kemeny's constant for the corresponding random walks coincide with the value of Kemeny's constant for the random walk on  $\mathcal{T}$ . Several illustrative examples are included.

**Key words.** Kemeny's constant, Stochastic matrix, Random walk on a graph.

**AMS subject classifications.** 05C50, 15B51, 60J10.

**1. Introduction.** An  $n \times n$  entrywise nonnegative matrix  $M$  is *stochastic* provided that each of its row sums is 1. Stochastic matrices are central to the study of discrete time, time-homogeneous, finite state space Markov chains. In particular, it is well-known that if the stochastic matrix  $M$  is *irreducible* – i.e., for each pair of distinct vertices  $u, v$  in the directed graph associated with  $M$  there is a directed path from  $u$  to  $v$  – then  $M$  has a unique *stationary distribution*, that is, a positive vector  $w$  whose entries sum to 1 such that  $w^\top M = w^\top$  (see [15], for example). Evidently 1 is an eigenvalue of  $M$ , and when  $M$  is irreducible, the Perron-Frobenius theorem yields the fact that necessarily 1 is algebraically simple. For each  $j = 1, \dots, n$ ,  $w_j$  can be interpreted as the long-term probability the Markov chain is in state  $j$ ; thus, the stationary vector captures long-term information about the Markov chain.

One way to quantify the short-term properties of a Markov chain is via the stan-

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<sup>†</sup>Department of Mathematics, University of Manitoba, Winnipeg, MB, Canada (stephen.kirkland@umanitoba.ca). Research supported in part by an NSERC Discovery Grant.

<sup>‡</sup>Department of Civil Engineering, University of Manitoba, Winnipeg, MB, Canada (zengz3@icloud.com). Research supported by a University of Manitoba Faculty of Science Undergraduate Summer Research Award.

dard notion of *mean first passage times*: for each  $i, j = 1, \dots, n$ , the mean first passage time  $e_{i,j}$  is the expected number of steps needed for the Markov chain to enter state  $j$  for the first time, given that the chain started in state  $i$ . Denoting the mean first passage matrix by  $E = [e_{i,j}]_{i,j=1}^n$ , the all-ones vector by  $\mathbf{1}$ , and the eigenvalues of  $M$  by  $1, \lambda_2, \dots, \lambda_n$ , we have the following remarkable result (see [8]):

$$Ew = \left( 1 + \sum_{j=2}^n \frac{1}{1 - \lambda_j} \right) \mathbf{1}.$$

In other words, the quantity  $\sum_{j=1}^n e_{i,j} w_j$ , which is the expected number of steps required to arrive at a random state (chosen according to the stationary distribution  $w$ ) starting from state  $i$ , is independent of  $i$ . The quantity  $\mathcal{K}(M) \equiv \sum_{j=2}^n \frac{1}{1 - \lambda_j}$  is known as *Kemeny's constant* for the Markov chain with transition matrix  $M$ , and it has been the subject of some research in recent years; see, for example [7], [9], [10], [11] and [13]. In particular, in a model for vehicle traffic networks based on Markov chains, Kemeny's constant has been used to measure the average travel time in the network [6]. In the present paper, Kemeny's constant is our main focus.

One of the most accessible families of Markov chains is the collection of random walks on undirected graphs: given a connected graph  $\mathcal{G}$  with  $(0, 1)$  adjacency matrix  $A$ , the transition matrix of the random walk on  $\mathcal{G}$  is given by  $D^{-1}A$ , where  $D = \text{diag}(A\mathbf{1})$ . It is readily verified that the stationary distribution for such a random walk is given by  $\frac{1}{d^T \mathbf{1}} d$ , where  $d$  is the degree vector for  $\mathcal{G}$  (equivalently,  $d = A\mathbf{1}$ ). Intuitively, one might expect that inserting an edge to a graph would necessarily decrease the value of Kemeny's constant for the corresponding random walk, but as we shall see in Section 3, there are examples of graphs where, surprisingly, inserting an edge can increase the value of Kemeny's constant. This is reminiscent of Braess' paradox for traffic networks, which we now briefly describe. In [1] (or see [2] for an English translation), Braess analyses a certain model for vehicle traffic on a road network, and presents an example in which the introduction of a road in the network actually increases the travel times for vehicles in the network. In view of the analogue between travel times on a road network and Kemeny's constant for a random walk on a graph, we make the following definition. Suppose that  $\mathcal{G}$  is a connected non-complete graph, and that  $e$  is an edge not in  $\mathcal{G}$ . We say that  $e$  is a *Braess edge* for  $\mathcal{G}$  if the value of Kemeny's constant for the random walk on  $\mathcal{G} \cup e$  exceeds that for the random walk on  $\mathcal{G}$ . We pursue this notion more deeply in Section 3.

Our work in Sections 3 and 4 focuses specifically on random walks on trees. This is a natural class of Markov chains to consider, partly because trees are the family of minimally connected graphs, and partly because in that setting, the graph-theoretic expression for Kemeny's constant (given in Theorem 3.1) is particularly transparent. By investigating Kemeny's constant for random walks on trees as a case study, we

hope to stimulate further research in the area.

Throughout the paper, we assume familiarity with basic material on directed and undirected graphs, stochastic matrices, and Markov chains. We refer the reader to [4], [8] and [15] for the necessary background.

**2. Preliminaries.** In this section, we present a few preliminary results that will assist us later. As noted in Section 1, we will focus on trees in Sections 3 and 4, and we recall the following terminology from [14]. Given a tree  $\mathcal{T}$ , recall that a *branch* at a vertex  $v$  of  $\mathcal{T}$  is a maximal subtree containing  $v$  as a pendent vertex. A *limb* at  $v$  is the union of one or more branches at  $v$ . Given a rooted tree  $\mathcal{R}$  we say that a tree  $\mathcal{T}$  has  $\mathcal{R}$  as a limb if there is a vertex  $v$  of  $\mathcal{T}$  and limb  $\mathcal{L}$  at  $v$  such that i)  $\mathcal{L}$  is isomorphic to  $\mathcal{R}$ , and ii) the isomorphism from  $\mathcal{L}$  to  $\mathcal{R}$  maps  $v$  to the root of  $\mathcal{R}$ . In Sections 3 and 4, we will use the following remarkable result due to Schwenk, which appears as Theorem 7 in [14].

PROPOSITION 2.1. *Let  $\mathcal{L}$  be any rooted tree. Then almost all trees have  $\mathcal{L}$  as a limb.*

We pause here to clarify the phrase ‘almost all’ in Proposition 2.1: Letting  $t_n$  denote the number of trees on  $n$  vertices, and  $r_n$  denote the number of trees on  $n$  vertices that do not have  $\mathcal{L}$  as a limb, then the content of Proposition 2.1 is that  $\lim_{n \rightarrow \infty} \frac{r_n}{t_n} = 0$ . We adopt similar phrasing in Theorems 3.6 and 4.2 below.

Next we introduce some useful terminology and notation. For an  $n \times n$  matrix  $B$ , for each  $j = 1, \dots, n$ , we let  $B_{(j)}$  denote the submatrix of order  $n - 1$  formed by deleting the  $j$ -th row and column. Similarly, for distinct indices  $j, k$  with  $1 \leq j, k \leq n$  we let  $B_{(j,k)}$  denote the submatrix of order  $n - 2$  formed by deleting the  $j$ -th and  $k$ -th rows and columns. Given a stochastic matrix  $M$  of order  $n$ , we define its *loop-free directed graph* to be the directed graph on vertices  $1, \dots, n$  such that for each pair of distinct indices  $j, k$  with  $1 \leq j, k \leq n$ , we include the directed arc  $j \rightarrow k$  if and only if  $m_{j,k} > 0$ . For any directed forest  $\mathcal{F}$  in the loop-free directed graph of  $M$ , we define the *weight* of  $\mathcal{F}$ ,  $w(\mathcal{F})$ , to be the product of the entries in  $M$  that correspond to the arcs in  $\mathcal{F}$ ; here we take the convention that if a tree consists of a single vertex, then its weight is 1. In the special case that we have a directed tree  $\mathcal{T}$  having a vertex  $v$  such that for any vertex  $u \neq v$  of  $\mathcal{T}$  there is a directed path from  $u$  to  $v$ , we refer to  $v$  as a *sink* for  $\mathcal{T}$ . (Such a directed tree is sometimes known as an *in-tree with root  $v$* .)

With this notation and terminology in place, we present the following result, which is an immediate consequence of the all-minors matrix tree theorem. We refer the interested reader to [3] for a proof of that theorem.

LEMMA 2.2. Let  $M$  be an irreducible stochastic matrix of order  $n \geq 3$ .

a) For each  $j = 1, \dots, n$ ,  $\det(I - M_{(j)}) = \sum_{\mathcal{T} \in S_j} w(\mathcal{T})$ , where  $S_j$  denotes the set of all spanning directed trees in the loop-free directed graph of  $M$  having vertex  $j$  as a sink.

b) For each  $j, k = 1, \dots, n$  with  $j \neq k$ ,  $\det(I - M_{(j,k)}) = \sum_{\mathcal{F} \in S_{j,k}} w(\mathcal{F})$ , where  $S_{j,k}$  is the set of all spanning directed forests in the loop-free directed graph of  $M$  such that each forest contains exactly two trees, one of which contains vertex  $j$  as a sink, and the other of which contains vertex  $k$  as a sink.

Lemma 2.2 is instrumental in the proof of the following result, which provides a combinatorial expression for Kemeny's constant. We note that a similar approach to individual mean first passage times appears in [5].

THEOREM 2.3. Let  $M$  be an irreducible stochastic matrix of order  $n \geq 3$ ,  $F_1$  be the set of all spanning directed trees in the loop-free directed graph of  $M$ , each of which has a vertex that is a sink, and  $F_2$  be the set of all spanning directed forests in the loop-free directed graph of  $M$  such that each forest consists of two trees, each of which has a vertex that is a sink. Then

$$(2.1) \quad \mathcal{K}(M) = \frac{\sum_{\mathcal{F} \in F_2} w(\mathcal{F})}{\sum_{\mathcal{T} \in F_1} w(\mathcal{T})}.$$

*Proof.* Denote the eigenvalues of  $M$  by  $1, \lambda_2, \dots, \lambda_n$ , and write the characteristic polynomial of  $I - M$  as  $f(x) = \det(xI - I + M) \equiv \sum_{j=0}^{n-1} f_j x^{n-j}$ . Evidently  $f_{n-1} = (-1)^{n-1}(1 - \lambda_2) \cdots (1 - \lambda_n)$ , and

$$f_{n-2} = (-1)^{n-2} \sum_{l=2}^n \frac{(1 - \lambda_2) \cdots (1 - \lambda_n)}{(1 - \lambda_l)} = -f_{n-1} \sum_{l=2}^n \frac{1}{(1 - \lambda_l)}.$$

We thus deduce that  $\mathcal{K}(M) = -\frac{f_{n-2}}{f_{n-1}}$ .

Next we recall that

$$f_{n-1} = (-1)^{n-1} \sum_{j=1}^n \det(I - M_{(j)}) \text{ and } f_{n-2} = (-1)^{n-2} \sum_{1 \leq j < k \leq n} \det(I - M_{(j,k)}).$$

Hence,

$$\mathcal{K}(M) = \frac{\sum_{1 \leq j < k \leq n} \det(I - M_{(j,k)})}{\sum_{j=1}^n \det(I - M_{(j)})},$$

and (2.1) now follows readily from Lemma 2.2 .  $\square$

If our stochastic matrix  $M$  is sparse (or nicely structured), then the sets  $F_1$  and  $F_2$  may be readily analysed in order to produce  $\mathcal{K}(M)$  via Theorem 2.3. The following example illustrates.

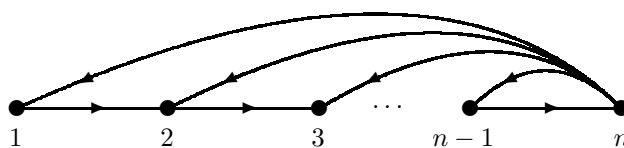


FIG. 2.1. Loop-free directed graph for a stochastic companion matrix.

EXAMPLE 2.1. Here we consider a stochastic companion matrix  $C$  given by

$$C = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 \\ \vdots & & \ddots & \ddots & & \vdots \\ 0 & 0 & \cdots & 0 & 1 & 0 \\ 0 & 0 & \cdots & 0 & 0 & 1 \\ c_1 & c_2 & c_3 & \cdots & c_{n-1} & c_n \end{bmatrix},$$

where  $c_1 > 0$  (in order to ensure irreducibility),  $c_j \geq 0, j = 2, \dots, n$  and  $\sum_{j=1}^n c_j = 1$ . Figure 2.1 illustrates the general form of the loop-free directed graph associated with  $C$ . (Note that for a particular given  $C$ , some of the arcs  $n \rightarrow j$  in Figure 2.1 may be absent, depending on which of the  $c_j$ s are positive.) Our goal is to find  $\mathcal{K}(C)$  by using Theorem 2.3.

First we consider the directed trees in  $\mathcal{F}_1$  in that theorem. For each  $j = 1, \dots, n - 1$ , the directed trees in  $\mathcal{F}_1$  with vertex  $j$  as a sink are of the form  $j + 1 \rightarrow j + 2 \rightarrow \cdots \rightarrow n \rightarrow l \cup 1 \rightarrow 2 \rightarrow \cdots \rightarrow j$ , where  $1 \leq l \leq j$ ; observe that such a directed tree has weight  $c_l$ . There is just one directed tree in  $\mathcal{F}_1$  having vertex  $n$  as a sink, namely  $1 \rightarrow 2 \rightarrow \cdots \rightarrow n$ , which has weight 1. Consequently we find that  $\sum_{\mathcal{T} \in \mathcal{F}_1} w(\mathcal{T}) = \sum_{j=1}^n \sum_{l=1}^j c_l = \sum_{k=1}^n (n - k + 1)c_k$ .

Next we consider the directed forests in  $\mathcal{F}_2$  in Theorem 2.3. Fix a pair of distinct vertices  $i, j$  where without loss of generality  $i < j$ . The directed forests in  $\mathcal{F}_2$  with vertices  $i$  and  $j$  as sinks are of two types:

- i) for each vertex  $l$  with  $1 \leq l \leq i$ , the directed forest  $\mathcal{T}_1 \cup \mathcal{T}_2$  where  $\mathcal{T}_1$  is  $j + 1 \rightarrow j + 2 \rightarrow \cdots \rightarrow n \rightarrow l \rightarrow l + 1 \rightarrow \cdots \rightarrow i \cup 1 \rightarrow 2 \rightarrow \cdots \rightarrow l$  and  $\mathcal{T}_2 = i + 1 \rightarrow i + 2 \rightarrow \cdots \rightarrow j$ ; and
- ii) for each vertex  $l$  with  $i + 1 \leq l \leq j$ , the directed forest  $\mathcal{T}_1 \cup \mathcal{T}_2$  where  $\mathcal{T}_1$  is

$j + 1 \rightarrow j + 2 \rightarrow \dots \rightarrow n \rightarrow l \rightarrow l + 1 \rightarrow \dots \rightarrow j \cup i + 1 \rightarrow 2 \rightarrow \dots \rightarrow l$  and  $\mathcal{T}_2 = 1 \rightarrow 2 \rightarrow \dots \rightarrow i$ .

Observe that the weight of each such directed forest is  $c_l$ . It now follows that the sum of the weights of the directed forests in  $\mathcal{F}_2$  with vertices  $i$  and  $j$  as sinks is  $\sum_{l=1}^j c_l$ . Hence,  $\sum_{\mathcal{F} \in \mathcal{F}_2} w(\mathcal{F}) = \sum_{1 \leq i < j \leq n} \sum_{l=1}^j c_l = \sum_{k=1}^n \frac{(n-k+1)(n+k-2)}{2} c_k$ .

Applying Theorem 2.3, it now follows that

$$\mathcal{K}(C) = \frac{\sum_{k=1}^n \frac{(n-k+1)(n+k-2)}{2} c_k}{\sum_{k=1}^n (n-k+1) c_k}.$$

In particular we see that  $\mathcal{K}(C)$  is a weighted average of the numbers  $\frac{n-1}{2}, \frac{n}{2}, \frac{n+1}{2}, \dots, \frac{2n-2}{2}$ . We thus deduce that for any stochastic companion matrix  $C$  of order  $n$ , we have

$$(2.2) \quad \frac{n-1}{2} \leq \mathcal{K}(C) \leq n-1.$$

The lower bound in (2.2) is attained when  $c_1 = 1$ , while the upper bound in (2.2) can be approached arbitrarily closely by taking each  $c_j, j = 1, \dots, n-1$  sufficiently close to 0.

For the special case of a random walk on an undirected graph, we have the following consequence of Theorem 2.3.

**COROLLARY 2.4.** *Suppose that  $\mathcal{G}$  is a connected, undirected graph on  $n$  vertices with degree sequence  $d_1, \dots, d_n$ . For each  $j, k = 1, \dots, n$  with  $j \neq k$ , let  $\sigma_{j,k}$  denote the number of spanning forests consisting of two trees, one of which contains vertex  $j$  and the other of which contains vertex  $k$ ; set  $\sigma_{j,j} = 0, j = 1, \dots, n$ . Let  $\tau$  be the number of spanning trees in  $G$ ,  $m$  denote the number of edges in  $\mathcal{G}$ , and let  $\Sigma$  be the matrix given by  $\Sigma = [\sigma_{j,k}]_{j,k=1}^n$ . Finally, let  $M$  be the transition matrix for the random walk on  $\mathcal{G}$ . Then*

$$\mathcal{K}(M) = \frac{d^\top \Sigma d}{4m\tau}.$$

*Proof.* Let  $S_j$  and  $S_{j,k}$  be as in Lemma 2.2. Fix an index  $j = 1, \dots, n$  and observe that any directed tree in  $S_j$  is formed by taking an undirected spanning tree in  $\mathcal{G}$  and orienting every arc so that  $j$  is a sink, and vice-versa. Further, for each directed tree  $\mathcal{T} \in S_j, w(\mathcal{T}) = \frac{d_j}{\prod_{l=1}^n d_l}$ . It now follows that

$$\sum_{j=1}^n \sum_{\mathcal{T} \in S_j} w(\mathcal{T}) = \frac{1}{\prod_{l=1}^n d_l} \sum_{j=1}^n d_j \tau = \frac{2m\tau}{\prod_{l=1}^n d_l}.$$

Similarly, note that whenever  $j, k = 1, \dots, n$  with  $j \neq k$ , each directed forest in  $S_{j,k}$  is formed by taking a spanning forest in  $\mathcal{G}$  consisting of two trees, one of which contains  $j$  and the other containing  $k$ , and orienting the arcs so that  $j$  and  $k$  are sinks in their respective trees. Each such forest has weight  $\frac{d_j d_k}{\prod_{l=1}^n d_l}$ , and it follows that

$$\sum_{1 \leq j < k \leq n} \sum_{\mathcal{F} \in S_{j,k}} w(\mathcal{F}) = \frac{1}{\prod_{l=1}^n d_l} \sum_{1 \leq j < k \leq n} d_j d_k |S_{j,k}| = \frac{d^\top \Sigma d}{2 \prod_{l=1}^n d_l}.$$

The conclusion now follows from Theorem 2.3.  $\square$

**3. Almost all trees have a Braess edge.** In this section, we focus on random walks on undirected trees. The section's key result, Theorem 3.5, shows that for any tree with a pair of *twin pendent* vertices – i.e., pendent vertices with a common neighbour – then inserting the edge between the twin pendent vertices increases the value of Kemeny's constant for the corresponding random walk. Given an undirected graph  $\mathcal{G}$ , we abuse notation slightly by using  $\mathcal{K}(\mathcal{G})$  to denote Kemeny's constant for the transition matrix of the random walk on  $\mathcal{G}$ .

The following result applies Corollary 2.4 to produce a particularly simple expression for  $\mathcal{K}(\mathcal{T})$  when  $\mathcal{T}$  is a tree.

**THEOREM 3.1.** *Suppose that  $\mathcal{T}$  is a tree on vertices  $1, \dots, n$  with degree sequence  $d_1, \dots, d_n$  and distance matrix  $\Delta = [\delta_{i,j}]_{i,j=1}^n$ . Then  $\mathcal{K}(\mathcal{T}) = \frac{d^\top \Delta d}{4(n-1)}$ .*

*Proof.* Referring to Corollary 2.4, it suffices to show that  $\delta_{j,k} = \sigma_{j,k}$  whenever  $j \neq k$ . Observe that each spanning forest in  $\mathcal{T}$  consisting of two trees is formed from  $\mathcal{T}$  by deleting precisely one edge. Evidently such a forest  $\mathcal{F}$  has vertex  $j$  in one tree and vertex  $k$  in the other if and only if the edge deleted to form  $\mathcal{F}$  is on the path between  $j$  and  $k$  in  $\mathcal{T}$ . It now follows that  $\delta_{j,k} = \sigma_{j,k}$  whenever  $j \neq k$ .  $\square$

The following trio of technical results will assist in the proof of Theorem 3.5. As usual  $e_j$  will denote a standard unit basis vector with a single 1 in the  $j$ -th position and zeros elsewhere; the order will always be clear from the context.

**LEMMA 3.2.** *Let  $\mathcal{T}$  be a tree on  $n \geq 3$  vertices with twin pendent vertices 1 and 2, both adjacent to vertex  $i$ . Let  $\tilde{\mathcal{T}}$  be the tree formed from  $\mathcal{T}$  by deleting vertices 1 and 2 as well as both incident edges. Denote the degree vectors and distance matrices for  $\mathcal{T}$  and  $\tilde{\mathcal{T}}$  by  $d, \Delta, \tilde{d}$ , and  $\tilde{\Delta}$ , respectively.*

a) *We have  $d^\top \Delta d = \tilde{d}^\top \tilde{\Delta} \tilde{d} + 8e_{i-2}^\top \tilde{\Delta} \tilde{d} + 8n - 12$ .*

b) *Let  $\mathcal{U}$  be the graph formed from  $\mathcal{T}$  by inserting the edge between vertices 1 and 2. Denote the degree vector for  $\mathcal{U}$  by  $\hat{d}$  and let  $\Sigma$  be as in Corollary 2.4. Then  $\hat{d}^\top \Sigma \hat{d} = 3\tilde{d}^\top \tilde{\Delta} \tilde{d} + 36e_{i-2}^\top \tilde{\Delta} \tilde{d} + 32n - 48$ .*



c) We have

$$\mathcal{K}(\mathcal{U}) - \mathcal{K}(\mathcal{T}) = \frac{-3\tilde{d}^\top \tilde{D}\tilde{d} + 12(n-3)e_{i-2}\tilde{\Delta}\tilde{d} + 4(n-4)(2n-3)}{12n(n-1)}.$$

*Proof.* a) Observe that we can write  $d^\top = [ 1 \quad 1 \mid \tilde{d}^\top + 2e_{i-2}^\top ]$  and

$$\Delta = \left[ \begin{array}{cc|c} 0 & 2 & (e_{i-2}^\top \tilde{\Delta} + \mathbf{1}^\top) \\ 2 & 0 & (e_{i-2}^\top \tilde{\Delta} + \mathbf{1}^\top) \\ \hline (\tilde{\Delta}e_{i-2} + \mathbf{1}) & (\tilde{\Delta}e_{i-2} + \mathbf{1}) & \tilde{\Delta} \end{array} \right].$$

Hence, we have

$$\Delta d = \left[ \begin{array}{c} 2 + e_{i-2}^\top \tilde{\Delta}\tilde{d} + 2(n-3) + 2 \\ 2 + e_{i-2}^\top \tilde{\Delta}\tilde{d} + 2(n-3) + 2 \\ \hline 2(\tilde{\Delta}e_{i-2} + \mathbf{1}) + \tilde{\Delta}\tilde{d} + 2\tilde{\Delta}e_{i-2} \end{array} \right].$$

It now follows that

$$d^\top \Delta d = 2(e_{i-2}^\top \tilde{\Delta}\tilde{d} + 2n - 2) + \tilde{d}^\top \tilde{\Delta}\tilde{d} + 4\tilde{d}^\top \tilde{\Delta}e_{i-2} + 2(2(n-3)) + 2e_{i-2}^\top \tilde{\Delta}\tilde{d} + 4,$$

which readily yields the conclusion.

b) Since the graph  $\mathcal{U}$  is unicyclic with a single cycle of length 3, we find that  $\sigma_{j,k} = 3\tilde{\delta}_{j,k}$  for each  $j, k = 3, \dots, n$ . Note also that  $\sigma_{1,2} = \sigma_{2,1} = 2$ . For each  $j = 3, \dots, n$  we have  $\sigma_{1,j} = 3\tilde{\delta}_{i-2,j} + 2$ , since this counts the number of forests in  $S_{1,j}$  such that 1,  $i$  are in the same tree, plus the number of forests in  $S_{1,j}$  such that 1,  $i$  are in different trees. From the above we find that

$$\Sigma = \left[ \begin{array}{cc|c} 0 & 2 & (3e_{i-2}^\top \tilde{\Delta} + 2\mathbf{1}^\top) \\ 2 & 0 & (3e_{i-2}^\top \tilde{\Delta} + 2\mathbf{1}^\top) \\ \hline (3\tilde{\Delta}e_{i-2} + 2\mathbf{1}) & (3\tilde{\Delta}e_{i-2} + 2\mathbf{1}) & 3\tilde{\Delta} \end{array} \right].$$

It is straightforward to determine that  $\hat{d}^\top = [ 2 \quad 2 \mid \tilde{d}^\top + 2e_{i-2}^\top ]$ . A computation now reveals that  $\hat{d}^\top \Sigma \hat{d} = 3\tilde{d}^\top \tilde{\Delta}\tilde{d} + 36e_{i-2}\tilde{\Delta}\tilde{d} + 32n - 48$ , as desired.

c) Since  $\mathcal{U}$  is unicyclic with a single cycle of length 3, it has  $n$  edges and 3 spanning trees. From Corollary 2.4 and part b) of the present lemma we thus have

$$\mathcal{K}(\mathcal{U}) = \frac{3\tilde{d}^\top \tilde{\Delta}\tilde{d} + 36e_{i-2}\tilde{\Delta}\tilde{d} + 32n - 48}{12n}.$$

From Theorem 3.1 and part a) of this lemma,

$$\mathcal{K}(\mathcal{T}) = \frac{\tilde{d}^\top \tilde{\Delta}\tilde{d} + 8e_{i-2}^\top \tilde{\Delta}\tilde{d} + 8n - 12}{4(n-1)}.$$

A computation now yields the desired expression for  $\mathcal{K}(\mathcal{U}) - \mathcal{K}(\mathcal{T})$ .  $\square$

In the next lemma and elsewhere, we use the following notation: for a graph  $\mathcal{G}$  with vertices  $u, v$  we denote the edge between  $u$  and  $v$  by  $u \sim v$ .

LEMMA 3.3. *Let  $\mathcal{T}$  be a tree on  $n \geq 2$  vertices with distance matrix  $\Delta$  and degree vector  $d$ . For each  $i, j = 1, \dots, n$ , we have*

$$(3.1) \quad e_j^\top \Delta d - e_i^\top \Delta d + 2n\delta_{i,j} \geq 4\delta_{i,j}.$$

*Proof.* We begin by noting that certainly (3.1) holds when  $\delta_{i,j} = 0$  – i.e., when  $i = j$ . To establish (3.1) when  $\delta_{i,j} \geq 1$ , We proceed by induction on  $\delta_{i,j}$ .

Suppose first that  $\delta_{i,j} = 1$ ; let  $C_1, C_2$  denote the connected components of  $\mathcal{T} \setminus \{i \sim j\}$ , where  $C_1$  has say  $p$  vertices and  $C_2$  has  $n - p$  vertices. Reordering indices if necessary so that those of  $C_1$  precede those of  $C_2$ , we find that there are vectors  $x, y \in \mathbb{R}^p, y \in \mathbb{R}^{n-p}$  such that

$$\begin{bmatrix} e_i^\top \Delta \\ e_j^\top \Delta \end{bmatrix} = \left[ \begin{array}{c|c} x^\top & y^\top + \mathbf{1}^\top \\ \hline x^\top + \mathbf{1}^\top & y^\top \end{array} \right].$$

It now follows that

$$(e_j - e_i)^\top \Delta d = \sum_{l \in C_1} d_l - \sum_{l \in C_2} d_l = 2(p - 1) + 1 - (2(n - p - 1) + 1) = 4p - 2n.$$

Hence,  $e_j^\top \Delta d - e_i^\top \Delta d + 2n\delta_{i,j} = 4p \geq 4 = 4\delta_{i,j}$ .

Fix  $k \geq 1$  and suppose now that (3.1) holds for pairs of vertices at distance  $k$ , and that  $\delta_{i,j} = k + 1$ . Select a vertex  $l \neq i, j$  that is on the path from  $j$  to  $i$ , and note that  $\delta_{j,l}, \delta_{l,i} \leq k$ . We have  $e_j^\top \Delta d - e_i^\top \Delta d + 2n\delta_{i,j} = (e_j^\top \Delta d - e_l^\top \Delta d + 2n\delta_{l,j}) + (e_l^\top \Delta d - e_i^\top \Delta d + 2n\delta_{i,l})$ . Applying the induction hypothesis to the pairs  $j, l$  and  $i, l$ , we have  $e_j^\top \Delta d - e_l^\top \Delta d + 2n\delta_{l,j} \geq 4\delta_{l,j} + 4\delta_{l,i} = 4\delta_{i,j}$ . This completes the proof of the induction step.  $\square$

LEMMA 3.4. *Let  $\mathcal{T}$  be a tree on  $n \geq 2$  vertices with degree vector  $d$  and distance matrix  $\Delta$ . For each  $i = 1, \dots, n$ , we have*

$$(3.2) \quad -d^\top \Delta d + 4(n - 1)e_i^\top \Delta d \geq 2(n - 1).$$

*Proof.* We proceed by induction on  $n$ . Note that when  $n = 2, d^\top = [1 \quad 1], \Delta = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ , in which case (3.2) is immediate.

Suppose now that (3.2) holds for trees on  $n \geq 2$  vertices, and that  $\mathcal{T}$  has  $n + 1$  vertices. Without loss of generality we take 1 as a pendent vertex, adjacent to vertex 2. Let  $\tilde{\mathcal{T}}$  denote the tree formed from  $\mathcal{T}$  by deleting vertex 1 and its incident edge; let  $\tilde{d}, \tilde{\Delta}$  denote the degree vector and distance matrix for  $\tilde{\mathcal{T}}$ , respectively. It is straightforward to see that  $d^\top = [1 \mid \tilde{d}^\top + \mathbf{1}^\top]$  and

$$\Delta = \left[ \begin{array}{c|c} 0 & e_1^\top \tilde{\Delta} + \mathbf{1}^\top \\ \hline \tilde{\Delta} e_1 + \mathbf{1} & \tilde{\Delta} \end{array} \right].$$

From this we find that

$$\Delta d = \left[ \begin{array}{c} e_1^\top \tilde{\Delta} \tilde{d} + 2n - 1 \\ \tilde{\Delta} \tilde{d} + 2\tilde{\Delta} e_1 + \mathbf{1} \end{array} \right].$$

It now follows that  $d^\top \Delta d = \tilde{d}^\top \tilde{\Delta} \tilde{d} + 4e_1^\top \tilde{\Delta} \tilde{d} + 4n - 2$ . Consequently,

$$\begin{aligned} & -d^\top \Delta d + 4ne_i^\top \Delta d \\ &= -\tilde{d}^\top \tilde{\Delta} \tilde{d} - 4e_1^\top \tilde{\Delta} \tilde{d} - 4n + 2 + 4n \begin{cases} e_1^\top \tilde{\Delta} \tilde{d} + 2n - 1, & \text{if } i = 1, \\ e_{i-1}^\top \tilde{\Delta} \tilde{d} + 2e_{i-1}^\top \tilde{\Delta} e_1 + 1, & \text{if } i = 2, \dots, n. \end{cases} \end{aligned}$$

In the case that  $i = 1$ , we find from (3.3) that

$$\begin{aligned} -d^\top \Delta d + 4ne_1^\top \Delta d &= -\tilde{d}^\top \tilde{\Delta} \tilde{d} - 4e_1^\top \tilde{\Delta} \tilde{d} - 4n + 2 + 4ne_1^\top \tilde{\Delta} \tilde{d} + 4n(2n - 1) \\ &= -\tilde{d}^\top \tilde{\Delta} \tilde{d} + 4(n - 1)e_1^\top \tilde{\Delta} \tilde{d} + 2(2n - 1)^2. \end{aligned}$$

Applying the induction hypothesis to  $\tilde{\mathcal{T}}$ , we now find that  $-d^\top \Delta d + 4ne_1^\top \Delta d \geq 2(n - 1) + 2(2n - 1)^2 > 2n$ .

In the case that  $i \geq 2$ , (3.3) yields

$$\begin{aligned} -d^\top \Delta d + 4ne_i^\top \Delta d &= -\tilde{d}^\top \tilde{\Delta} \tilde{d} - 4e_1^\top \tilde{\Delta} \tilde{d} - 4n + 2 + 4n(e_{i-1}^\top \tilde{\Delta} \tilde{d} + 2e_{i-1}^\top \tilde{\Delta} e_1 + 1) \\ &= -\tilde{d}^\top \tilde{\Delta} \tilde{d} + 4(n - 1)e_{i-1}^\top \tilde{\Delta} \tilde{d} + 2 + 4(e_{i-1}^\top \tilde{\Delta} \tilde{d} - e_1^\top \tilde{\Delta} \tilde{d} + 2n\tilde{\delta}_{i-1,1}). \end{aligned}$$

From Lemma 3.3 we have  $e_{i-1}^\top \tilde{\Delta} \tilde{d} - e_1^\top \tilde{\Delta} \tilde{d} + 2n\tilde{\delta}_{i-1,1} \geq 4\tilde{\delta}_{i-1,1} \geq 0$ , and from the induction hypothesis applied to  $\tilde{\mathcal{T}}$  we have  $-\tilde{d}^\top \tilde{\Delta} \tilde{d} + 4(n - 1)e_{i-1}^\top \tilde{\Delta} \tilde{d} \geq 2(n - 1)$ . Assembling the above it now follows that  $-d^\top \Delta d + 4ne_i^\top \Delta d \geq 2(n - 1) + 2 = 2n$ . This completes the proof of the induction step.  $\square$

**REMARK 3.1.** Examining the proof of Lemma 3.4, we find that equality can hold in (3.2) only in the case that  $n = 2$  or vertex  $i$  is adjacent to the particular pendent vertex selected at the start of the proof of the induction step. But since the pendent vertex initially selected was arbitrary, we deduce that when  $n \geq 3$ , equality can hold in (3.2) only if vertex  $i$  is adjacent to every pendent vertex – i.e.,  $\mathcal{T}$  is the star in  $n$  vertices  $\mathcal{K}_{1,n-1}$ , with  $i$  as the centre vertex.

We now present one of the main results of this section.

**THEOREM 3.5.** *Let  $\mathcal{T}$  be a tree on  $n \geq 3$  vertices with twin pendent vertices 1 and 2. Let  $\mathcal{U}$  be the graph formed from  $\mathcal{T}$  by inserting the edge between vertices 1 and 2. Then*

$$(3.3) \quad \mathcal{K}(\mathcal{U}) - \mathcal{K}(\mathcal{T}) \geq \frac{4n - 15}{6n}.$$

*Proof.* From Lemma 3.2,

$$\mathcal{K}(\mathcal{U}) - \mathcal{K}(\mathcal{T}) = \frac{-3\tilde{d}^\top \tilde{D}\tilde{d} + 12(n-3)e_{i-2}\tilde{\Delta}\tilde{d} + 4(n-4)(2n-3)}{12n(n-1)},$$

where  $\tilde{d}$  and  $\tilde{\Delta}$  are the degree vector and distance matrix for the tree  $\tilde{\mathcal{T}}$  on  $n-2$  vertices formed from  $\mathcal{T}$  by deleting vertices 1 and 2 and their incident edges. By Lemma 3.4,  $-\tilde{d}^\top \tilde{D}\tilde{d} + 4(n-3)e_{i-2}\tilde{\Delta}\tilde{d} \geq 2(n-3)$ , so that  $\mathcal{K}(\mathcal{U}) - \mathcal{K}(\mathcal{T}) \geq \frac{4n^2 - 19n + 15}{6n(n-1)} = \frac{4n-15}{6n}$ , as desired.  $\square$

**REMARK 3.2.** Examining the proof of Theorem 3.5, we find the equality holds in (3.3) only if it holds in (3.2) (for vertex  $i-2$  in  $\tilde{\mathcal{T}}$ ). Referring to Remark 3.1 we find that the latter holds only when  $\tilde{\mathcal{T}}$ , and hence,  $\mathcal{T}$  is a star. It now follows readily that equality holds in (3.3) if and only if  $\mathcal{T} = \mathcal{K}_{1,n-1}$ .

We have the following ‘Schwenk-type’ result.

**THEOREM 3.6.** *For almost every tree  $\mathcal{T}$ , there is a Braess edge for  $\mathcal{T}$ .*

*Proof.* According to Proposition 2.1, given any rooted tree  $\mathcal{L}$ , almost all trees contain  $\mathcal{L}$  as a limb. In particular, we find that almost all trees contain a pair of twin pendent vertices. The conclusion now follows from Theorem 3.5.  $\square$

The following example considers the effect of inserting a weighted edge to the star  $\mathcal{K}_{1,n-1}$ .

**EXAMPLE 3.1.** Suppose that  $n \geq 4$  and consider the weighted graph  $\mathcal{U}(h)$  formed from  $\mathcal{K}_{1,n-1}$  by inserting a single edge of weight  $h > 0$  between two pendent vertices. Letting  $M(h)$  denote the transition matrix for the random walk on  $\mathcal{U}(h)$ , we can write  $M(h)$  as

$$M(h) = \left[ \begin{array}{cc|cc} 0 & \frac{h}{1+h} & 0^\top & \frac{1}{1+h} \\ \frac{h}{1+h} & 0 & 0^\top & \frac{1}{1+h} \\ \hline 0 & 0 & 0 & \mathbf{1} \\ \hline \frac{1}{n-1} & \frac{1}{n-1} & \frac{1}{n-1}\mathbf{1}^\top & 0 \end{array} \right].$$

The eigenvalues of  $M(h)$  are: 1 with multiplicity one; 0 with multiplicity  $n-4$ ;

$-\frac{h}{1+h}$ ; and  $-\frac{1}{2(1+h)} \pm \sqrt{\frac{1}{4(1+h)^2} + \frac{h(n-3)}{(1+h)(n-1)}}$ , these last three having multiplicity one. A sequence of computations shows that  $\mathcal{K}(M(h)) = n - \frac{3}{2} + \frac{h(4(n-3)h-3)}{(2h+1)(2h+2(n-1))}$ . It now follows that  $\mathcal{K}(M(h)) < \mathcal{K}(\mathcal{K}_{1,n-1})$  for  $0 < h < \frac{3}{4(n-3)}$ ,  $\mathcal{K}(M(h)) = \mathcal{K}(\mathcal{K}_{1,n-1})$  for  $h = \frac{3}{4(n-3)}$ , and  $\mathcal{K}(M(h)) > \mathcal{K}(\mathcal{K}_{1,n-1})$  for  $h > \frac{3}{4(n-3)}$ .

Set  $g(h) = \frac{h(4(n-3)h-3)}{(2h+1)(2h+2(n-1))}$ , and let

$$h_0 = \frac{-4(n-3)(n-1) + \sqrt{16(n-3)^2(n-1)^2 + 3(n-1)(8n^2 - 28n + 18)}}{8n^2 - 28n + 18}.$$

An elementary exercise reveals that  $\mathcal{K}(M(h))$  is decreasing on the interval  $h \in (0, h_0)$  and increasing on the interval  $(h_0, \infty)$ .

We have the following structural result for trees.

**PROPOSITION 3.7.** *Suppose that  $\mathcal{T}$  is a tree on  $n \geq 3$  vertices. Then  $\mathcal{T}$  has a next to pendent vertex of degree 2, or it has a pair of twin pendent vertices.*

*Proof.* We proceed by induction on  $n$ , and note that when  $n = 3$ , the tree in question has both types of vertices.

Suppose now that  $n \geq 4$ , and that the statement holds for trees on  $n - 1$  vertices. Let  $\mathcal{T}$  be a tree on  $n$  vertices, say with vertex 1 as a pendent vertex adjacent to vertex 2. Let  $\overline{\mathcal{T}} = \mathcal{T} \setminus \{1\}$ ; for clarity, the vertices in  $\overline{\mathcal{T}}$  inherit their labels from  $\mathcal{T}$ . Consider vertex 2 of  $\overline{\mathcal{T}}$  and denote its degree in  $\overline{\mathcal{T}}$  by  $d$ . If  $d = 1$ , then in  $\mathcal{T}$  vertex 2 is a next to pendent vertex of degree 2. Suppose now that  $d \geq 2$ . From the induction hypothesis, there is a vertex  $i$  of  $\overline{\mathcal{T}}$  such that either  $i$  is next to pendent and of degree 2 in  $\overline{\mathcal{T}}$ , or there are two pendent vertices of  $\overline{\mathcal{T}}$  that are adjacent to  $i$ . If  $i \geq 3$ , then considered as a vertex of  $\mathcal{T}$ , vertex  $i$  has the corresponding desired property. If  $i = 2$  and there are two pendent vertices of  $\overline{\mathcal{T}}$  adjacent to 2, then the same is true in  $\mathcal{T}$ . If in  $\overline{\mathcal{T}}$  we have that vertex 2 is adjacent to a pendent vertex  $j$ , then in  $\mathcal{T}$ , 1 and  $j$  are pendent vertices both adjacent to vertex 2. Thus, in all cases,  $\mathcal{T}$  has the desired property, completing the proof of the induction step.  $\square$

From Proposition 3.7, any tree has either a pair of twin pendent vertices, or a pendent vertex adjacent to a vertex of degree 2. Theorem 3.5 shows that creating a three-cycle by inserting an edge between twin pendent vertices in a tree with at least 4 vertices will increase the value of Kemeny's constant. Our next two examples show that creating a three-cycle by inserting the edge between the two neighbours of a next to pendent of degree 2 may raise or lower the value of Kemeny's constant, depending on the structure of the original tree.

**EXAMPLE 3.2.** Here we consider the tree  $\mathcal{T}$  on  $n \geq 5$  vertices formed from the star  $\mathcal{K}_{1,n-3}$  by appending a path of length two at the centre vertex. The corresponding

distance matrix can be written as

$$\left[ \begin{array}{c|c|c|c} 0 & 1 & \mathbf{31}^\top & 2 \\ \hline 1 & 0 & \mathbf{21}^\top & 1 \\ \hline \mathbf{31} & \mathbf{21} & 2(J-I) & \mathbf{1} \\ \hline 2 & 1 & \mathbf{1}^\top & 0 \end{array} \right].$$

It now follows from Theorem 3.1 that  $\mathcal{K}(\mathcal{T}) = \frac{2n^2-n-9}{2(n-1)}$ .

Next, we form the graph  $\mathcal{U}$  by inserting the edge between vertex 1 and vertex  $n$ . Using the technique of Lemma 3.2 b), we find that  $\mathcal{K}(\mathcal{U}) = \frac{6n^2-5n-15}{6n}$ . It now follows that

$$\mathcal{K}(\mathcal{U}) - \mathcal{K}(\mathcal{T}) = \frac{-8n^2 + 17n + 15}{6n(n-1)},$$

which is negative since  $n \geq 5$ .

EXAMPLE 3.3. Suppose that  $n \geq 4$ , and consider the path on  $n$  vertices  $\mathcal{P}_n$ , with vertices labelled so that vertex  $j$  is adjacent to vertices  $j-1, j+1$  for  $j = 2, \dots, n-1$ . We have degree vector  $d = [1 \ 2 \ \dots \ 2 \ 1]^\top$  and distance matrix  $\Delta = [ |i-j| ]_{i,j=1}^n$ . A computation using Theorem 3.1 now shows that  $\mathcal{K}(\mathcal{P}_n) = \frac{2n^2-4n+3}{6}$ . Next we form the unicyclic graph  $\mathcal{U}_n$  by inserting the edge  $1 \sim 3$  to  $\mathcal{P}_n$ . Applying the technique of Lemma 3.2 b) it follows that  $\mathcal{K}(\mathcal{U}_n) = \frac{2n^3-37n+81}{6n}$ . Consequently,

$$\mathcal{K}(\mathcal{U}_n) - \mathcal{K}(\mathcal{P}_n) = \frac{4n^2 - 40n + 81}{6n},$$

which is positive for all  $n \geq 8$ .

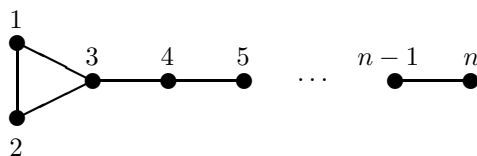


FIG. 3.1.  $\mathcal{U}_n$ .

REMARK 3.3. Consider the unicyclic graph  $\mathcal{U}_n$  depicted in Figure 3.1. Note that the only edges that can be deleted from  $\mathcal{U}_n$  while maintaining connectivity are the edges  $1 \sim 2$ ,  $2 \sim 3$ , and  $1 \sim 3$ . From Example 3.3, we see that if  $n \geq 8$ , then deleting either  $2 \sim 3$  or  $1 \sim 3$  will lower the corresponding value of Kemeny's constant, while by Theorem 3.5, deleting  $1 \sim 2$  will also lower the corresponding value of Kemeny's

constant. Thus, for  $n \geq 8$ ,  $\mathcal{U}_n$  has the intriguing property that the effect of deleting any edge is to either destroy connectivity or decrease the corresponding value of Kemeny's constant.

The graph  $U_n$  in Figure 3.1 is a member of the family of so-called *lollipop graphs*, each of which is constructed from a cycle of length  $k \geq 3$  by appending a path on  $n - k \geq 1$  vertices. Figure 3.2 illustrates. Our next example examines Kemeny's constant for the family of lollipop graphs on a fixed number of vertices.

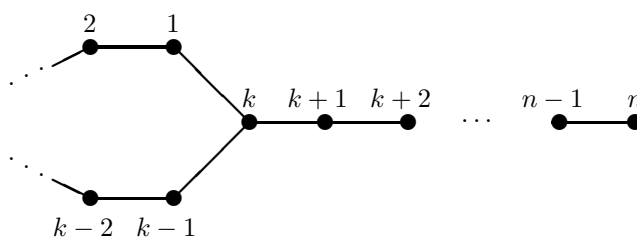


FIG. 3.2. The lollipop graph  $\mathcal{L}_{k,n}$ .

EXAMPLE 3.4. Observe that each lollipop graph can be constructed from the path  $\mathcal{P}_n$  (where the vertices have been labelled so that vertex  $j$  is adjacent to vertices  $j - 1$  and  $j + 1$  for each  $j = 2, \dots, n - 1$ ) by inserting the edge  $1 \sim k$  for some  $3 \leq k \leq n - 1$ . Our goal in this example is to derive an expression for Kemeny's constant for the lollipop graph on  $n$  vertices with cycle length  $k$ , then examine that expression as a function of  $k$ . To that end, fix an index  $k$  with  $3 \leq k \leq n - 1$ , and consider the corresponding lollipop graph  $\mathcal{L}_{k,n}$ , labelled as in Figure 3.2. Observe that the degree vector  $d$  can be written as  $d = [2 \ 2 \ \dots \ 2 \ 3 \ 2 \ 2 \ \dots \ 2 \ 1]^T$ , where the lone 3 appears in the  $k$ -th position. We adopt the notation of Corollary 2.4, and use this to derive expressions for  $\sigma_{i,j}, i, j = 1, \dots, n$ .

Suppose first that  $i, j \in \{1, \dots, k\}$ . Each forest in  $S_{i,j}$  is generated by deleting one edge from each of the two paths that connect  $i$  and  $j$  on the  $k$ -cycle. Consequently,  $\sigma_{i,j} = |j - i|(k - |j - i|)$  when  $i, j \in \{1, \dots, k\}$ .

Next, suppose that  $i, j \in \{k + 1, \dots, n\}$ . Each forest in  $S_{i,j}$  is generated by deleting one edge on the path between  $i$  and  $j$ , and one edge on the  $k$ -cycle. Hence,  $\sigma_{i,j} = k|j - i|$  when  $i, j \in \{k + 1, \dots, n\}$ .

Finally, suppose that  $i \in \{1, \dots, k\}$  and  $j \in \{k + 1, \dots, n\}$ . Each forest in  $S_{i,j}$  is generated either by deleting one edge from each of the two paths that connect  $i$  and  $k$  on the  $k$ -cycle, or by deleting one edge on the path between  $k$  and  $j$ , and one edge

on the  $k$ -cycle. We thus find that  $\sigma_{i,j} = i(k - i) + k(j - k)$  when  $i \in \{1, \dots, k\}, j \in \{k + 1, \dots, n\}$ .

A long and not especially interesting computation now shows that  $d^\top \Sigma d = \left(\frac{2k}{3}\right) (2n^3 - 4nk^2 + 3k^3 - n)$ . Appealing to Corollary 2.4, we find that

$$(3.4) \quad \mathcal{K}(\mathcal{L}_{k,n}) = \frac{2n^3 - 4nk^2 + 3k^3 - n}{6n}.$$

We note in passing that for the  $n$ -cycle  $\mathcal{C}_n$  we have  $\mathcal{K}(\mathcal{C}_n) = \frac{n^2-1}{6}$ , so that (3.4) also holds in the case  $k = n$ , provided that we accept the natural interpretation that  $\mathcal{L}_{n,n} = \mathcal{C}_n$ . Considered as a function of  $k$ , it is straightforward to determine that  $\frac{2n^3 - 4nk^2 + 3k^3 - n}{6n}$  is decreasing in  $k$  for  $3 \leq k \leq \frac{8n}{9}$  and increasing in  $k$  for  $\frac{8n}{9} \leq k \leq n$ . Thus, we have the somewhat surprising result that  $\mathcal{K}(\mathcal{L}_{k,n})$  fails to be monotonically decreasing in  $k$  when  $n \geq 10$ .

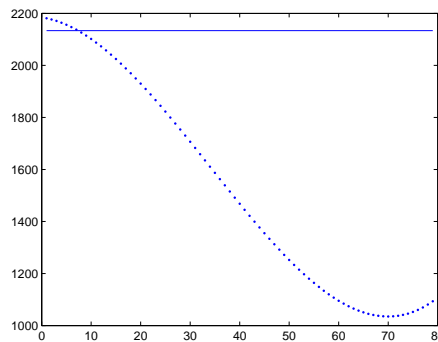


FIG. 3.3. *Kemeny's constants for lollipop graphs on 81 vertices.*

We have already seen from Example 3.3 that  $\mathcal{K}(\mathcal{L}_{3,n}) > \mathcal{K}(\mathcal{P}_n)$ . For which values of  $k$  do we have  $\mathcal{K}(\mathcal{L}_{k,n}) \leq \mathcal{K}(\mathcal{P}_n)$ ? Referring to Example 3.3, we find that the inequality  $\mathcal{K}(\mathcal{L}_{k,n}) \leq \mathcal{K}(\mathcal{P}_n)$  can be rewritten as

$$\frac{2n^3 - 4nk^2 + 3k^3 - n}{6n} \leq \frac{2n^2 - 4n + 3}{6}.$$

This last is readily seen to simplify to the condition

$$p(k) \equiv 3k^3 - 4nk^2 + 4n^2 - 4n \leq 0.$$

Since  $p(k)$  is decreasing in  $k$  on the interval  $[0, \frac{8n}{9}]$  and increasing on  $[\frac{8n}{9}, n]$ , and since  $p(n) < 0 < p(0)$ , we deduce that there is precisely one  $k_0 \in [0, n]$  such that  $p(k_0) = 0$ , and that  $p(k) > 0$  for  $0 \leq k < k_0$  and  $p(k) < 0$  for  $k_0 < k \leq n$ . Evidently



$p(\sqrt{n}) = (3\sqrt{n} - 4)n > 0$ , so that necessarily  $\sqrt{n} < k_0$ . Another computation shows that  $p(\sqrt{n} + \frac{3}{8}) = -\frac{19}{16}n + \frac{27}{64}\sqrt{n} + \frac{81}{512}$ , which is readily seen to be negative since  $n \geq 4$ . Hence, we have  $k_0 < \sqrt{n} + \frac{3}{8}$ . Consequently, we find that there is a  $k_0 \in (\sqrt{n}, \sqrt{n} + \frac{3}{8})$  such that  $\mathcal{K}(\mathcal{L}_{k,n}) \geq \mathcal{K}(\mathcal{P}_n)$  for  $3 \leq k \leq k_0$  and  $\mathcal{K}(\mathcal{L}_{k,n}) \leq \mathcal{K}(\mathcal{P}_n)$  for  $k_0 \leq k \leq n$ .

Figure 3.3 plots  $\mathcal{K}(\mathcal{L}_{k,81})$  (as computed by Matlab<sup>®</sup>) for the values  $k = 3, \dots, 81$ , again interpreting the  $k = 81$  case as  $\mathcal{C}_{81}$ ; the horizontal line in Figure 3.3 is at height  $\mathcal{K}(\mathcal{P}_{81}) = 2133.5$ . Observe that the minimum value for  $\mathcal{K}(\mathcal{L}_{k,81})$  corresponds to  $k = 72$ , and that  $\mathcal{K}(\mathcal{L}_{9,81}) > \mathcal{K}(\mathcal{P}_{81}) > \mathcal{K}(\mathcal{L}_{10,81})$ , as anticipated by our discussion in this example.

**4. Almost all trees have many co-Kemeny mates.** We say that two connected nonisomorphic graphs  $\mathcal{G}_1, \mathcal{G}_2$  on the same number of vertices are *co-Kemeny mates* if  $\mathcal{K}(\mathcal{G}_1) = \mathcal{K}(\mathcal{G}_2)$ . In this section, we again focus on trees, but this time we consider the issue of co-Kemeny mates.

Recall that for a connected undirected graph  $\mathcal{G}$  with adjacency matrix  $A$  and diagonal matrix of vertex degrees  $D$ , the *normalised Laplacian matrix* for  $\mathcal{G}$  is given by  $L = I - D^{-\frac{1}{2}}AD^{-\frac{1}{2}}$ ; it is straightforward to see that  $I - L$  is diagonally similar to the transition matrix of the random walk on  $\mathcal{G}$ . In particular, we observe that if the normalised Laplacian matrices for two graphs have the same spectra, then so do the transition matrices of the corresponding random walks. A result of Osborne [12] states that for almost every tree  $\mathcal{T}$ , there is another tree  $\hat{\mathcal{T}}$  which is not isomorphic to  $\mathcal{T}$ , but which has the same normalised Laplacian spectrum as  $\mathcal{T}$ . From our observation above, it follows immediately that almost all trees have a co-Kemeny mate. The main result of this section, Theorem 4.2, proves a stronger result regarding co-Kemeny mates, namely that given any  $m \in \mathbb{N}$ , almost all trees have at least  $m$  co-Kemeny mates.

The following technical result allows us to compare the value of Kemeny's constant for two related trees.

**PROPOSITION 4.1.** *Consider a tree  $\mathcal{T}_0$  with two distinct vertices  $i$  and  $j$ , and let  $\mathcal{B}$  be another tree rooted at vertex  $k$ . Form  $\mathcal{T}_1$  from  $\mathcal{T}_0$  and  $\mathcal{B}$  by inserting an edge between vertex  $i$  of  $\mathcal{T}_0$  and vertex of  $k$  of  $\mathcal{B}$ ; form  $\mathcal{T}_2$  from  $\mathcal{T}_0$  and  $\mathcal{B}$  by inserting an edge between vertex  $j$  of  $\mathcal{T}_0$  and vertex of  $k$  of  $\mathcal{B}$ . Let  $d(1), \Delta(1)$  denote the degree vector and distance matrix for  $\mathcal{T}_1$ , and let  $d(2), \Delta(2)$  denote the degree vector and distance matrix for  $\mathcal{T}_2$ .*

*Denote the path in  $\mathcal{T}_0$  from  $i$  to  $j$  by  $i \equiv l_0 \sim l_1 \sim \dots \sim l_d \equiv j$ . Let  $C_0$  denote the component of  $\mathcal{T}_0 \setminus \{l_0 \sim l_1\}$  containing vertex  $l_0$ , let  $C_d$  denote the component of  $\mathcal{T}_0 \setminus \{l_{d-1} \sim l_d\}$  containing vertex  $l_d$ , and for each  $p = 1, \dots, d - 1$ , let  $C_p$  denote the component of  $\mathcal{T}_0 \setminus \{l_{p-1} \sim l_p, l_p \sim l_{p+1}\}$  containing vertex  $l_p$ .*

Then

$$(4.1) \quad d(1)^\top \Delta(1)d(1) - d(2)^\top \Delta(2)d(2) = 8|\mathcal{B}| \sum_{j=0}^d |C_j|(2j - d).$$

*Proof.* Denote the degree vectors and distance matrices for  $\mathcal{B}$  and  $\mathcal{T}_0$  by  $d_{\mathcal{B}}$ ,  $d_{\mathcal{T}_0}$ ,  $\Delta_{\mathcal{B}}$ , and  $\Delta_{\mathcal{T}_0}$ , respectively. Then  $d(1)^\top = [d_{\mathcal{B}}^\top + e_k^\top \mid d_{\mathcal{T}_0}^\top + e_i^\top]$ , and

$$\Delta(1) = \left[ \begin{array}{c|c} \Delta_{\mathcal{B}} & \Delta_{\mathcal{B}}e_k\mathbf{1}^\top + \mathbf{1}e_i^\top\Delta_{\mathcal{T}_0} + J \\ \hline \mathbf{1}e_k^\top\Delta_{\mathcal{B}} + \Delta_{\mathcal{T}_0}e_i\mathbf{1}^\top + J & \Delta_{\mathcal{T}_0} \end{array} \right],$$

where  $J$  denotes an all ones matrix. Consequently we find that

$$\begin{aligned} d(1)^\top \Delta(1)d(1) &= (d_{\mathcal{B}}^\top + e_k^\top)\Delta_{\mathcal{B}}(d_{\mathcal{B}} + e_k) + (d_{\mathcal{T}_0}^\top + e_i^\top)\Delta_{\mathcal{T}_0}(d_{\mathcal{T}_0} + e_i) \\ &\quad + 2(d_{\mathcal{B}}^\top + e_k^\top)(\Delta_{\mathcal{B}}e_k\mathbf{1}^\top + \mathbf{1}e_i^\top\Delta_{\mathcal{T}_0} + J)(d_{\mathcal{T}_0} + e_i). \end{aligned}$$

An analogous expression holds for  $d(2)^\top \Delta(2)d(2)$ , and it now follows that

$$\begin{aligned} &d(1)^\top \Delta(1)d(1) - d(2)^\top \Delta(2)d(2) \\ &= 2e_i^\top \Delta_{\mathcal{T}_0} d_{\mathcal{T}_0} + 2(2|\mathcal{B}| - 1)e_i^\top \Delta_{\mathcal{T}_0} d_{\mathcal{T}_0} - 2e_j^\top \Delta_{\mathcal{T}_0} d_{\mathcal{T}_0} - 2(2|\mathcal{B}| - 1)e_j^\top \Delta_{\mathcal{T}_0} d_{\mathcal{T}_0} \\ &= 4|\mathcal{B}|(e_i^\top - e_j^\top)\Delta_{\mathcal{T}_0} d_{\mathcal{T}_0}. \end{aligned}$$

Fix an index  $p$  with  $0 \leq p \leq d$ , and suppose that  $q \in C_p$ . Then for some integer  $r$  we have  $e_i^\top \Delta_{\mathcal{T}_0} e_q = r + p$  and  $e_j^\top \Delta_{\mathcal{T}_0} e_q = r + d - p$ , so that  $(e_i^\top - e_j^\top)\Delta_{\mathcal{T}_0} e_q = 2p - d$ . If  $p = 0$  or  $d$  we have  $\sum_{q \in C_p} e_q^\top d_{\mathcal{T}_0} = 2(|C_j| - 1) + 1 = 2|C_j| - 1$ , while for  $p = 1, \dots, d - 1$ ,  $\sum_{q \in C_p} e_q^\top d_{\mathcal{T}_0} = 2(|C_p| - 1) + 2 = 2|C_p|$ . Consequently we find that

$$(e_i^\top - e_j^\top)\Delta_{\mathcal{T}_0} d_{\mathcal{T}_0} = -d(2|C_0| - 1) + d(2|C_d| - 1) + \sum_{p=1}^{d-1} 2|C_p|(2p - d) = 2 \sum_{p=0}^d |C_p|(2p - d).$$

The expression (4.1) now follows.  $\square$

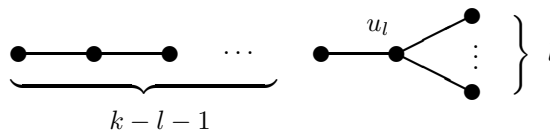


FIG. 4.1.  $\mathcal{T}_{k,l}$ .

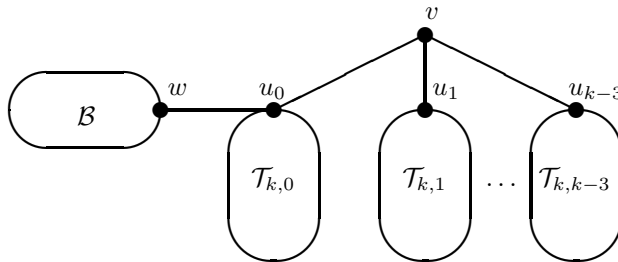


FIG. 4.2. The tree  $\mathcal{R}_0(k)$  for Example 4.1.

The following example produces families of trees which are all co-Kemeny mates.

EXAMPLE 4.1. For each  $k \geq 4$  and  $1 \leq l \leq k - 3$ , let  $\mathcal{T}_{k,l}$  be the rooted tree on  $k$  vertices, formed from the star  $\mathcal{K}_{1,l}$  (rooted at the centre vertex, which we label as  $u_l$ ) by appending a path on  $k - l - 1$  vertices at the root vertex  $u_l$ . (This type of tree is sometimes known as a ‘broom’.) We define  $\mathcal{T}_{k,0}$  to be the path  $\mathcal{P}_k$  with root  $u_0$  at one end point of the path. Figure 4.1 illustrates. Next we form a tree  $\mathcal{L}_k$  from  $\cup_{l=0}^{k-3} \mathcal{T}_{k,l}$  by inserting a new vertex  $v$ , and making it adjacent to each of the roots vertices  $u_0, \dots, u_{k-3}$ . Observe that in  $\mathcal{L}_k$ , for each  $l = 0, \dots, k - 3$ , vertex  $u_l$  has degree  $l + 2$ .

Fix a  $k \geq 4$ , and take any tree  $\mathcal{B}$ , rooted at vertex  $w$ , say. For each  $l = 0, \dots, k - 3$ , form the tree  $\mathcal{R}_l(k)$  from  $\mathcal{B} \cup \mathcal{L}_k$  by inserting the edge between  $w$  and  $u_l$ . (Here we are suppressing the explicit dependence on  $\mathcal{B}$ .) Denote the corresponding degree vector and distance matrix by  $d(l), \Delta(l)$ , respectively. Figure 4.2 illustrates  $\mathcal{R}_0(k)$ .

We claim that  $d(l_1)^\top \Delta(l_1) d(l_1) = d(l_2)^\top \Delta(l_2) d(l_2)$  whenever  $0 \leq l_1 < l_2 \leq k - 3$ . To see the claim, observe that Proposition 4.1 applies. In the language and notation of that proposition, the path from  $u_{l_1}$  to  $u_{l_2}$  is  $u_{l_1} \sim v \sim u_{l_2}$ , so that  $d = 2$ . Observe also that  $|C_0| = k, |C_1| = 1$  and  $|C_2| = k$ . According to (4.1) we have

$$d(l_1)^\top \Delta(l_1) d(l_1) - d(l_2)^\top \Delta(l_2) d(l_2) = 8|\mathcal{B}|(k(0 - 2) + 1(2 - 2) + k(4 - 2)) = 0,$$

as claimed. For each  $k \geq 4$  and each  $l = 0, \dots, k - 3$ , we find from Theorem 3.1 and the preceding observations that  $\mathcal{K}(\mathcal{R}_0(k)) = \mathcal{K}(\mathcal{R}_1(k)) = \dots = \mathcal{K}(\mathcal{R}_{k-3}(k))$ . We note that the trees  $\mathcal{R}_l(k), l = 0, \dots, k - 3$  are nonisomorphic, since they all have different degree sequences.

The following remark shows that in addition to being nonisomorphic, many of the trees in Example 4.1 fail to be cospectral with respect to the transition matrix of the corresponding random walk.

REMARK 4.1. Fix a  $k \geq 4$  and an  $l$  with  $0 \leq l \leq k - 3$ , and denote the transition

matrix for the random walk on  $\mathcal{R}_l(k)$  by  $M_l(k)$ . It is straightforward to determine that, denoting the degree vector of  $\mathcal{R}_l(k)$  by  $d$ , we have  $\text{trace}((M_l(k))^2) = 2 \sum_{p \sim q} \frac{1}{d_p d_q}$ . Observe that this sum can be separated into two pieces – a sum over edges incident with  $u_l$ , and a sum over edges not incident with  $u_l$ . This yields

$$\text{trace}((M_l(k))^2) = 2 \sum_{p \sim q, p, q \neq u_l} \frac{1}{d_p d_q} + 2 \sum_{p \sim u_l} \frac{1}{d_p d_{u_l}} = 2 \sum_{p \sim q, p, q \neq u_l} \frac{1}{d_p d_q} + \frac{2}{l+3} \sum_{p \sim u_l} \frac{1}{d_p}.$$

Observe that for  $l = 0, \dots, k-3$ ,  $\sum_{p \sim u_l} \frac{1}{d_p} = l + \frac{1}{2} + \frac{1}{d_w} + \frac{1}{k-2}$ .

Suppose that we have indices  $l_1, l_2$  with  $0 \leq l_1 < l_2 \leq k-3$ . We want to compute  $\text{trace}((M_{l_1}(k))^2) - \text{trace}((M_{l_2}(k))^2)$ ; we do so by considering, for each of  $\mathcal{R}_{l_1}(k)$  and  $\mathcal{R}_{l_2}(k)$ , edges incident with  $u_{l_1}$ , edges incident with  $u_{l_2}$ , and edges incident with neither  $u_{l_1}$  nor  $u_{l_2}$ . It now follows that

$$\begin{aligned} & \frac{1}{2} (\text{trace}((M_{l_1}(k))^2) - \text{trace}((M_{l_2}(k))^2)) \\ &= \frac{1}{l_1+3} \left( l_1 + \frac{1}{2} + \frac{1}{d_w} + \frac{1}{k-2} \right) + \frac{1}{l_2+2} \left( l_2 + \frac{1}{2} + \frac{1}{k-2} \right) \\ & \quad - \frac{1}{l_2+3} \left( l_2 + \frac{1}{2} + \frac{1}{d_w} + \frac{1}{k-2} \right) - \frac{1}{l_1+2} \left( l_1 + \frac{1}{2} + \frac{1}{k-2} \right) \\ &= \left( -\frac{5}{2} + \frac{1}{d_w} + \frac{1}{k-2} \right) \left( \frac{1}{l_1+3} - \frac{1}{l_2+3} \right) + \left( -\frac{3}{2} + \frac{1}{k-2} \right) \left( \frac{1}{l_2+2} - \frac{1}{l_1+2} \right). \end{aligned}$$

Inspecting (4.2) we find readily that if  $d_w = 1$ , then

$$\text{trace}((M_{l_1}(k))^2) \neq \text{trace}((M_{l_2}(k))^2).$$

Suppose now that  $d_w \geq 2$ , and note that  $\text{trace}((M_{l_1}(k))^2) = \text{trace}((M_{l_2}(k))^2)$  if and only if

$$\left( \frac{3}{2} - \frac{1}{k-2} \right) \frac{(l_1+3)(l_2+3)}{(l_1+2)(l_2+2)} = \frac{5}{2} - \frac{1}{d_w} - \frac{1}{k-2}.$$

Observe that since  $l_2 \geq l_1 + 1$ ,  $\frac{(l_1+3)(l_2+3)}{(l_1+2)(l_2+2)} \leq \frac{(l_1+3)(l_1+4)}{(l_1+2)(l_1+3)} = \frac{l_1+4}{l_1+2}$ . If we suppose further that  $l_1 \geq 4$ , then  $\left( \frac{3}{2} - \frac{1}{k-2} \right) \frac{(l_1+3)(l_2+3)}{(l_1+2)(l_2+2)} \leq \left( \frac{3}{2} - \frac{1}{k-2} \right) \frac{l_1+4}{l_1+2} \leq \frac{4}{3} \left( \frac{3}{2} - \frac{1}{k-2} \right) = 2 - \frac{4}{3(k-2)}$ . Since  $d_w \geq 2$ , we have  $2 - \frac{1}{k-2} \leq \frac{5}{2} - \frac{1}{d_w} - \frac{1}{k-2}$ .

Assembling the observations above, we have that when  $d_w \geq 2$  and  $l_1 \geq 4$ ,

$$\left( \frac{3}{2} - \frac{1}{k-2} \right) \frac{(l_1+3)(l_2+3)}{(l_1+2)(l_2+2)} \leq 2 - \frac{4}{3(k-2)} < 2 - \frac{1}{k-2} \leq \frac{5}{2} - \frac{1}{d_w} - \frac{1}{k-2}.$$

In particular,  $\text{trace}((M_{l_1}(k))^2) \neq \text{trace}((M_{l_2}(k))^2)$  whenever  $l_1 \geq 4$ .

We thus conclude that the transition matrices  $M_l(k), l = 4, \dots, k - 3$ , (of which there are  $k - 6$ ) necessarily have distinct spectra.

Here is our final result, which is also of 'Schwenk-type'.

**THEOREM 4.2.** *Fix an  $m \in \mathbb{N}$ . Then almost all trees have at least  $m$  co-Kemeny mates, none of which are cospectral with respect to the transition matrix of the corresponding random walk.*

*Proof.* Choose  $k = m + 7$ . According to Proposition 2.1, for almost every tree  $\mathcal{T}$  there is a vertex  $w$  having  $\mathcal{L}_k$  as a branch at  $w$ , with  $w$  adjacent to  $u_0$ . From Example 4.1, we find that for each  $l = 1, \dots, k - 3$ , the tree formed from  $\mathcal{T}$  by deleting the edge  $w \sim u_0$  and inserting the edge  $w \sim u_l$  is a co-Kemeny mate for  $\mathcal{T}$ . Moreover, by Remark 4.1, at least  $k - 6 = m + 1$  of the trees so constructed have transition matrices with distinct spectra. Hence, at most one of those trees has the property that the spectrum of its transition matrix coincides with that of  $\mathcal{T}$ , which readily yields the conclusion.  $\square$

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