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Kemeny's constant and the effective graph resistance $\stackrel{\text{tr}}{\sim}$

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Abstract

Kemeny's constant and its relation to the effective graph resistance has been established for regular graphs by Palacios et al. [1]. Based on the Moore-Penrose pseudo-inverse of the Laplacian matrix, we derive a new closed-form formula and deduce upper and lower bounds for the Kemeny constant. Furthermore, we generalize the relation between the Kemeny constant and the effective graph resistance for a general connected, undirected graph.

Keywords: Kemeny constant, effective graph resistance or Kirchhoff index, multiplicative degree-Kirchhoff index, Moore-Penrose pseudo-inverse, spectral graph theory 2010 MSC: 15A09, 15A18, 15A63

1. Introduction

Consider an undirected graph G(N, L) with N nodes and L links. The adjacency matrix A of a graph G is an $N \times N$ symmetric matrix with elements a_{ij} that are either 1 or 0 depending on whether there is a link between nodes i and j or not. The Laplacian matrix Q of G is an $N \times N$ symmetric matrix $Q = \Delta - A$, where $\Delta = \text{diag}(d_i)$ is the $N \times N$ diagonal degree matrix with the elements $d_i = \sum_{j=1}^N a_{ij}$. Let $d = (d_1, d_2, \ldots, d_N)$ denote the degree vector for a graph G. The Laplacian eigenvalues of Q are all real and non-negative [2]. The eigenvalues of Q are ordered as $0 = \mu_N \leq \mu_{N-1} \leq \ldots \leq \mu_1$. For a connected graph, the second smallest eigenvalue, coined the algebraic connectivity by Fiedler [3], is positive, i.e., $\mu_{N-1} > 0$. The Laplacian matrix Q is not invertible due to a zero eigenvalue $\mu_N = 0$, but one of the generalized matrix inverses is the Moore-Penrose pseudo-inverse, denoted as Q^{\dagger} .

The effective graph resistance R_G , also called Kirchhoff index, characterizes the resistance distance [4] between nodes in an electrical network and can be computed by $R_G = N \sum_{i=1}^{N-1} \frac{1}{\mu_i}$, where μ_i is the i-th eigenvalue of the Laplacian matrix Q. Studies [5, 6, 7] relate the effective graph resistance and the trace of the pseudo-inverse Laplacian Q^{\dagger} as

$$R_G = N \text{trace}(Q^{\dagger}) = N \sum_{j=1}^{N} (Q^{\dagger})_{jj}$$

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Bounds and closed-form formulas for the effective graph resistance are extensively investigated in some classes of graphs, such as regular graphs [8], Cayley graphs [9] and circulant graphs [10]. In complex networks, represented by graphs, the effective graph resistance characterizes the difficulty of transport in a network. As a robustness indicator, the effective graph resistance allows to compare graphs and is applied in improving the robustness of complex networks, especially against cascading failures in electrical networks [11, 12, 13].

Let *P* denote the transition probability matrix of a finite, irreducible Markov Chain and the steady state probability vector π and the all-one vector *u* satisfying Pu = u and $\pi^T P = \pi^T$.

Theorem 1 ([14]). Let h and g be any two column vectors such that the scalar products $h^T u$ and $\pi^T g$ are nonzero. Then the inverse

$$Z \equiv \left(I - P + gh^T\right)^{-1}$$

exists.

The Kemeny constant is defined, in terms of the trace of the matrix Z, as

$$K(P) \equiv \operatorname{trace}\left(Z\right) - \pi^T Z u$$

For a given transition probability matrix P and with $h^T g = 1$, the Kemeny constant K(P) is the same regardless of the choice of the matrix Z defined in Theorem 1.

Kemeny offered a prize for the first person to find an intuitively plausible interpretation for his constant. Peter Doyle suggested the following explanation: *choose a target state j according to the steady state probability vector. Start from a state i and wait until the time* T_j , *also called hitting time, that the target state occurs for the first time. Let* X_k , $k \ge 0$ *denote the states of the Markov chain. The expected hitting time is* $E[T_j|X_0 = i] = 1 + \sum_{k \ne j} p_{ik}E[T_j|X_0 = k]$. By the *maximum principle* $E[T_j|X_0 = i]$ *is a constant.* The explanation is reported in the second edition (2003) of a book [15] by Grinstead and Snell along with a question "Should Peter have been given the prize?". An alternative interpretation is provided by Levene and Loizou [16]. Rewrite K(P)as $K(P) = \sum_{i=1}^{N} \pi_i \sum_{j=1}^{N} \pi_j m_{ij}$ in a finite irreducible Markov chain, where m_{ij} is the mean hitting time from a state *i* to a state *j* and π is the steady-state vector. Imagine a random surfer who is following links according to the transition probabilities. At some stage the random surfer does not know in which state he is and where he is heading. In this scenario, the Kemeny constant can be interpreted as the mean number of links the random surfer follows before reaching his destination.

Kirkland [17] studied the Kemeny constant K(P) via the group inverse of the matrix I - P for the directed graph associated with the transition matrix P. A closed-form expression [18] for the Kemeny constant was provided in terms of the weights of certain directed forests in a directed graph of matrix P. The Kemeny constant and its relation to the effective graph resistance R_G was previously investigated by Palacios et al. [8, 1, 19]. For a regular graph with degree r, the relation between the Kemeny constant and the effective graph resistance was shown to be

$$K(P) = \frac{r}{N}R_G$$

However, the relation between the Kemeny constant K(P) and the effective graph resistance R_G in a general graph is missing so far.

Motivated by advances of the pseudo-inverse of the Laplacian, such as its appearance in the electrical current flow equation [4], the relation with the effective resistance [2] in electrical networks, the relation with the mean first-passage time [20, 21] in a Markov-chain model of random walks and the state-of-the-art application in identifying the best spreader node [6] in a graph, we connect the Kemeny constant and the effective graph resistance via the pseudo-inverse of the Laplacian. The paper is organized as follows. Section 2 presents a new closed-form formula for the Kemeny constant. Bounds for the Kemeny constant and the relation to the effective graph resistance are derived in Section 3. Section 4 concludes the paper.

2. New closed-form formula for the Kemeny constant

The stochastic matrix $P = \Delta^{-1}A$ characterizes a random walk on a graph that is timereversible. One of the main contributions of this paper is Theorem 4, which derives a new closed-form formula for the Kemeny constant based on the pseudo-inverse of the Laplacian matrix. We first state two lemmas that will be used in the proof of Theorem 4.

Lemma 2. Consider the $N \times N$ transition probability matrix $P = \Delta^{-1}A$. The all-one column vector u satisfies Pu = u. The column vector $\pi = \frac{d}{2L}$ satisfies $\pi^T P = \pi^T$ and $\pi^T u = 1$. The Moore-Penrose pseudo-inverse of the matrix I - P equals,

$$(I - P)^{\dagger} = \left(I - P + \pi u^{T}\right)^{-1} - \frac{u\pi^{T}}{u^{T}u\pi^{T}\pi}$$
(1)

Proof. See Appendix A.

Lemma 3. The Moore-Penrose pseudo-inverse of the matrix product $\Delta^{-1}QQ^{\dagger}$ can be simplified as

$$\left(\Delta^{-1}QQ^{\dagger}\right)^{\dagger} = \Delta - \Delta \frac{dd^{T}}{d^{T}d}$$
⁽²⁾

where column vector d is the degree vector of a graph G and matrix Q is the Laplacian matrix.

Proof. See Appendix B

Theorem 4. Assume the transition probability matrix $P = \Delta^{-1}A$. A closed-form formula for the *Kemeny constant follows*

$$K(\Delta^{-1}A) = \zeta^T d - \frac{d^T Q^{\dagger} d}{2L}$$
(3)

where the column vector $\zeta = (Q_{11}^{\dagger}, Q_{22}^{\dagger}, \dots, Q_{NN}^{\dagger})$.

Proof. For the given transition matrix $P = \Delta^{-1}A$, all the matrices Z defined in Theorem 1 with $\beta^T g = 1$ result in the same Kemeny constant. Choose the matrix Z as

$$Z \equiv \left(I - P + \pi u^T\right)^{-1} \tag{4}$$

Lemma 2 shows that the Moore-Penrose pseudo-inverse of the matrix I - P can be rewritten in terms of matrix Z as

$$(I-P)^{\dagger} = Z - \frac{u\pi^{I}}{u^{T}u\pi^{T}\pi}$$
⁽⁵⁾

The Kemeny constant can be written as, with trace $\left(\frac{u\pi^T}{u^T u\pi^T \pi}\right) = \frac{4L^2}{Nd^T d}$,

$$K(\Delta^{-1}A) = \operatorname{trace}\left(Z\right) - \pi^{T}Zu = \operatorname{trace}\left((I-P)^{\dagger}\right) + \frac{4L^{2}}{Nd^{T}d} - \pi^{T}Zu$$
(6)

Next, we focus on the Moore-Penrose pseudo-inverse of the matrix I - P. Substituting $P = \Delta^{-1}A$, we have that

$$(I-P)^{\dagger} = \left(\Delta^{-1}(\Delta-A)\right)^{\dagger} = \left(\Delta^{-1}Q\right)^{\dagger}$$

In general, the pseudo-inverse of the product of two matrices does NOT follow the product of the pseudo-inverse of each matrix, i.e., $(AB)^{\dagger} \neq B^{\dagger}A^{\dagger}$, but [22]

$$(AB)^{\dagger} = \left(A^{\dagger}AB\right)^{\dagger} \left(ABB^{\dagger}\right)^{\dagger} \tag{7}$$

Let $A = \Delta^{-1}$ and B = Q, we arrive at

$$\left(\Delta^{-1}Q\right)^{\dagger} = Q^{\dagger} \left(\Delta^{-1}QQ^{\dagger}\right)^{\dagger}$$

According to lemma 3, matrix $(\Delta^{-1}QQ^{\dagger})^{\dagger}$ can be further simplified as

$$\left(\Delta^{-1}QQ^{\dagger}\right)^{\dagger} = \Delta - \Delta \frac{dd^{T}}{d^{T}d} \tag{8}$$

The Moore-Penrose pseudo-inverse of the matrix I - P thus follows

$$(I-P)^{\dagger} = Q^{\dagger} \Delta - Q^{\dagger} \Delta \frac{dd^{T}}{d^{T} d}$$
⁽⁹⁾

and the trace of $(I - P)^{\dagger}$ can be written as

trace
$$((I - P)^{\dagger})$$
 = trace $(Q^{\dagger}\Delta)$ - trace $(Q^{\dagger}\Delta \frac{dd^{T}}{d^{T}d})$ (10)

where trace $(Q^{\dagger}\Delta) = \sum_{i=1}^{N} (Q^{\dagger})_{ii} d_i = \zeta^T d$. With the inner product of two vectors following trace $(xy^T) = x^T y$, we have that

trace
$$\left(\frac{Q^{\dagger}\Delta d}{d^{T}d}d^{T}\right) = d^{T}\frac{\left(Q^{\dagger}\Delta\right)d}{d^{T}d}$$
 (11)

Substituting (10) into (6) yields

$$K(\Delta^{-1}A) = \zeta^T d - d^T \frac{\left(\mathcal{Q}^{\dagger}\Delta\right)d}{d^T d} + \frac{4L^2}{Nd^T d} - \pi^T Z u$$
(12)

Next, we focus on simplifying the term $\pi^T Z u$. After left multiplying π and right multiplying u of (5), we arrive at

$$\pi^{T} Z u = \pi^{T} \left(I - P \right)^{\dagger} u + \pi^{T} \frac{u \pi^{T}}{u^{T} u \pi^{T} \pi} u$$
(13)

4

Introducing the matrix $(I - P)^{\dagger}$ in (9) and with $\pi = \frac{d}{2L}$, we obtain that

$$\pi^T Z u = \frac{d^T Q^{\dagger} d}{2L} - \frac{d^T \left(Q^{\dagger} \Delta\right) d}{d^T d} + \frac{4L^2}{N d^T d}$$
(14)

Substituting (14) into (12), we establish Theorem 4.

Corollary 1. The Kemeny constant can be expressed, in terms of the effective resistance matrix Ω , as

$$K(\Delta^{-1}A) = \frac{d^T \Omega d}{4L}$$
(15)

where $\Omega = (\omega_{ij})$ and each element ω_{ij} represents the resistance on the link between nodes *i* and *j*.

Proof. The effective resistance matrix Ω can be written [2], in terms of the pseudo-inverse Laplacian, as

$$\Omega = \zeta u^T + u\zeta^T - 2Q^{\dagger} \tag{16}$$

Left multiplying d^T and right multiplying d yields

$$d^T \Omega d = 4L \zeta^T d - 2d^T Q^{\dagger} d \tag{17}$$

Dividing 4L on both sides of (17) and substituting to Theorem 4 results in (15). \Box

The Kemeny constant in (15) contains a quadratic form,

$$d^{T}\Omega d = \sum_{i=1}^{N} \sum_{j=1}^{N} d_{i}\omega_{ij}d_{j}$$
(18)

and each term $d_i \omega_{ij} d_j$ in a connected graph (with non-negative link weights) is positive: there is a path between each pair (i, j) of nodes with positive effective resistance and each node has, at least, a degree $d_i \ge 1$. Hence, Corollary 1 indicates that the Kemeny constant is strictly positive.

Theorem 4 enables the computation of K(P) via the pseudo-inverse of the Laplacian in the unweighted, undirected graph associated with the transition matrix P, which is different from the approach in [18] employing the weighted, directed graph of the matrix P. The result in Corollary 1 was obtained by Palacios and Renom [23, Corollary 1] working with a different Z matrix, $Z = (I - P + u\pi^T)^{-1}$, which is called the fundamental matrix [15]. Moreover, half of the quadratic form in (18) is also defined [24, 23] as the multiplicative degree-Kirchhoff index $R_G^* = \frac{1}{2}d^T\Omega d$. The Kemeny constant relates to R_G^* in the form of $K(\Delta^{-1}A) = \frac{R_G^*}{2L}$.

3. Generalization of the relation between $K(\Delta^{-1}A)$ and R_G

In this section, we derive a general relation between the Kemeny constant and the effective graph resistance. Sharp upper and lower bounds are deduced for the Kemeny constant. Finally, we study the Kemeny constant for special graphs.

3.1. Generalization of the relation

Corollary 2. Assume the probability transition matrix $P = \Delta^{-1}A$. The relation between the Kemeny constant $K(\Delta^{-1}A)$ and the effective graph resistance R_G is described as

$$\frac{d_{min}R_G}{N} - \frac{d^T Q^{\dagger} d}{2L} \le K(\Delta^{-1}A) \le \frac{d_{max}R_G}{N}$$
(19)

where d_{min} and d_{max} is the minimum and the maximum degree in graph G, respectively.

Proof. An inequality for the term $\zeta^T d$ in (3) follows

$$d_{\min}\zeta^T u \le \zeta^T d \le d_{\max}\zeta^T u \tag{20}$$

Substituting (20) into (3), together with $\zeta^T u = \frac{R_G}{N}$ and $\frac{d^T Q^{\dagger} d}{2L} \ge 0$ due to the positive semidefiniteness of the matrix Q^{\dagger} , we establish the general relation between $K(\Delta^{-1}A)$ and R_G , i.e., Corollary 2.

For a regular graph with degree r, the degree vector follows d = ru. Since $Q^{\dagger}u = 0$, the quadratic form for a regular graph follows

$$d^T Q^{\dagger} d = 0 \tag{21}$$

The Kemeny constant in Theorem 4 is reduced to $K(\Delta^{-1}A) = r\zeta^T u = r\frac{R_G}{N}$, which was found earlier by Palacios et al. [1].

Moreover, a sharper lower bound than that in (19) is presented by invoking a new lower bound for the term $\zeta^T d$. Applying the lower bound of Q_{ii}^{\dagger} , derived in [6],

$$Q_{ii}^{\dagger} \ge \frac{1}{d_i} \left(1 - \frac{1}{N} \right)^2 \tag{22}$$

to the term $\zeta^T d = \sum_{i=1}^N Q_{ii}^{\dagger} d_i$ yields

$$\zeta^T d \ge N \left(1 - \frac{1}{N} \right)^2$$

Combining with (3), a sharper lower bound for the Kemeny constant follows

$$K(\Delta^{-1}A) \ge N\left(1 - \frac{1}{N}\right)^2 - \frac{d^T Q^{\dagger} d}{2L}$$
(23)

Next, we show that a lower bound (24) for the effective graph resistance (or the Kirchhoff index) can be obtained by using (22). Invoking (22) and $R_G = N$ trace (Q^{\dagger}) , we arrive at

$$R_G \ge \frac{(N-1)^2}{N} \sum_{i=1}^N \frac{1}{d_i}$$

Employing the inequality $\sum_{i=1}^{N} \frac{1}{d_i} \ge \frac{N^2}{2L}$ in [25], we show that

$$R_G \ge \frac{N\left(N-1\right)^2}{2L} \tag{24}$$

The lower bound (24) is a pretty good bound obtained circa 2014-2015 (see, e.g., [12, 25, 26, 27]), but is superseded by the state-of-the-art result in [25, Theorem 1].

3.2. Bounds for Kemeny's constant

Since $Q^{\dagger}u = 0$, we rewrite the degree vector as

$$d = d_{av}u - \delta \tag{25}$$

where the average degree $d_{av} = \frac{2L}{N} = \frac{d^T u}{N}$. This definition (25) has two direct consequences. First,

$$\delta^T u = 0$$

implying that the difference vector of the degree has mean zero, is orthogonal to the vector $x_N = \frac{u}{\sqrt{N}}$ belonging to the zero Laplacian eigenvalue $\mu_N = 0$ and that δ can be written as a linear combination of all eigenvectors of the Laplacian (and pseudo-inverse Laplacian) belonging to positive eigenvalues (for a connected graph). Thus,

$$\delta = \sum_{k=1}^{N-1} \left(\delta^T x_k \right) x_k \tag{26}$$

which also illustrates that $\delta^T u = 0$ due to orthogonality of the Laplacian eigenvectors $x_k^T x_m = \delta_{km}$ (where δ_{km} is the Kronecker delta), because $x_N = \frac{u}{\sqrt{N}}$. Next, the norm $\|\delta\| = \sqrt{\delta^T \delta}$ follows from

$$\delta^{T}\delta = (d - d_{av}u)^{T} (d - d_{av}u) = d^{T}d - Nd_{av}^{2}$$
(27)

which also equals, invoking (26) and orthogonality of the eigenvectors,

$$\delta^T \delta = \sum_{k=1}^{N-1} \left(\delta^T x_k \right)^2$$

The stochastic interpretation is $\operatorname{Var}[D] = E\left[(D - E[D])^2\right] = E\left[D^2\right] - (E[D])^2 = \frac{d^Td}{N} - d_{av}^2$, where *D* is the random variable of the degree in a graph, which equals the degree of a randomly selected node in the graph.

After this preparation, we introduce the definition (25) into the quadratic form

$$d^T Q^{\dagger} d = \delta^T Q^{\dagger} \delta$$

due to $Q^{\dagger}u = 0$. Invoking the inequality [28, (5.4) on p. 99],

$$\frac{1}{\mu_1} \leq \frac{\delta^T Q^{\dagger} \delta}{\delta^T \delta} = \frac{\sum_{k=1}^{N-1} \frac{1}{\mu_k} \left(\delta^T x_k\right)^2}{\sum_{k=1}^{N-1} \left(\delta^T x_k\right)^2} \leq \frac{1}{\mu_{N-1}}$$

we find with (27) that

$$\frac{d^T d - N d_{av}^2}{\mu_1} \le \delta^T Q^{\dagger} \delta \le \frac{d^T d - N d_{av}^2}{\mu_{N-1}}$$
(28)

Consequently, the Kemeny constant $K(\Delta^{-1}A)$ in (3) is upper and lower bounded by

$$\zeta^{T}d - \frac{\operatorname{Var}[D]}{E[D]\mu_{N-1}} \le K(\Delta^{-1}A) \le \zeta^{T}d - \frac{\operatorname{Var}[D]}{E[D]\mu_{1}}$$
(29)

Involving $K(\Delta^{-1}A) = \frac{R_G^*}{2L}$, we derive upper and lower bounds for the multiplicative degree-Kirchhoff index

$$2L\zeta^{T}d - \frac{N\operatorname{Var}[D]}{\mu_{N-1}} \le R_{G}^{*} \le 2L\zeta^{T}d - \frac{N\operatorname{Var}[D]}{\mu_{1}}$$
(30)

which improves the lower bound in [29]

$$R_G^* \ge N - 1 + 2L(N - 2) \tag{31}$$

We numerically evaluate the upper and lower bounds in (29) for various random graphs. In Figure 1, we present the accuracy of the bounds for (a) Erdős-Rényi graphs (ER) with N = 500 nodes, link density $p = 2p_c$, where $p_c = \frac{\log(N)}{N}$ is the connectivity threshold; (b) Barabási-Albert graphs (BA) with N = 500 and the average degree $d_{av} = 6$; (c) Watts-Strogatz small-world graphs (WS) with N = 500, the average degree $d_{av} = 6$ and the rewiring probability p = 0.1. The generation of these random graphs is described in, e.g., [30] for ER graphs, [31] for BA graphs, and [32] for WS graphs. For each class of random graphs, we generate 10^5 graph instances and the probability density functions and the bounds for the Kemeny constant $K(\Delta^{-1}A)$ are plotted. The upper bound deviates on average 0.01%, 0.04% and 0.002% of the numerical value of the Kemeny constant in ER random graphs, BA graphs and WS graphs, respectively. The lower bound is slightly less accurate compared to the upper bound, with 0.05%, 0.8% and 0.04% of difference in ER, BA and WS graphs. Hence, the simulation results show that the upper and lower bounds in (29) are a good approximation for $K(\Delta^{-1}A)$. Moreover, Table 1 shows that the result (30) improves the lower bound for the multiplicative degree-Kirchhoff index found in [29].

Table 1: Accuracy of lower bounds (30) and (31) in random graphs with the same parameters as in Figure 1. The value in each column is the average value over 10^5 graph instances.

Random graphs	$R_G^*/2L$	lower bound (31)/2L	lower bound (30)/2L
ER graphs	544.38	498.08	544.11
BA graphs	603.87	498.17	598.80
WS graphs	949.97	498.17	949.54

3.3. Quadratic form $d^T Q^{\dagger} d$ in star graphs

The Laplacian for a star graph with N nodes can be written as

$$Q = \begin{bmatrix} N - 1 & -u_{1 \times (N-1)}^T \\ -u_{(N-1) \times 1}^T & I_{(N-1) \times (N-1)} \end{bmatrix}$$
(32)

The pseudo-inverse of the Laplacian matrix can be computed [2] by

$$Q^{\dagger} = (Q+J)^{-1} - \frac{J}{N^2}$$
(33)

where J is the all-one matrix. With (32), we can write the inverse of matrix Q + J as

$$(Q+J)^{-1} = \begin{bmatrix} N & 0\\ 0 & I+J \end{bmatrix}^{-1} = \begin{bmatrix} \frac{1}{N} & 0\\ 0 & I-\frac{J}{N} \end{bmatrix}$$
(34)



Figure 1: Accuracy of the upper and lower bounds for the Kemeny constant.

Left multiplying d^T and right multiplying d in (33), together with (34) and using d = (N - 1, 1, ..., 1), we have that $\frac{d^T Q^{\dagger} d}{2L} = \frac{1}{2} - \frac{2(N-1)}{N^2}$. From (3), the Kemeny constant for a star graph can be explicitly expressed as $K(\Delta^{-1}A) = N - \frac{3}{2}$. Due to $\zeta^T d = (N - 2)Q_{11}^{\dagger} + \frac{R_G}{N}$ and $Q_{11}^{\dagger} = \frac{N-1}{N^2}$, the Kemeny constant is rewritten, in terms of the effective graph resistance R_G , as

$$K(\Delta^{-1}A) = \frac{R_G}{N} + \frac{N-2}{2N}$$
(35)



(c) WS graphs with N = 500, $d_{av} = 6$ and rewiring probability p = 0.1

Figure 1: Accuracy of the upper and lower bounds for the Kemeny constant.

4. Conclusion

In this paper, we generalize the relation between the Kemeny constant and the effective graph resistance, which was known for regular graphs, to general connected, undirected graphs. By deriving a new closed-form formula (3), we provide a new approach to compute the Kemeny constant via the pseudo-inverse of the Laplacian matrix. Moreover, we show that for general graphs the Kemeny constant can be tightly upper and lower bounded by (29).

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Appendix A. Proof of Lemma 2

Proof. According to Theorem 1, the inverse matrix $Z = (I - P + \pi u^T)^{-1}$ exists. The definition of the inverse of a matrix reads

$$\left(I - P + \pi u^T\right) \left(I - P + \pi u^T\right)^{-1} = I \tag{A.1}$$

Left multiplying π^T in (A.1) yields, with $\pi^T P = \pi^T$,

$$u^T \left(I - P + \pi u^T \right)^{-1} = \frac{\pi^T}{\pi^T \pi}$$

Substituting into (A.1) results in

$$(I - P)(I - P + \pi u^{T})^{-1} = I - \frac{\pi \pi^{T}}{\pi^{T} \pi}$$

Similarly, the following can be obtained

$$(I - P + \pi u^{T})^{-1} (I - P) = I - \frac{u u^{T}}{u^{T} u}$$
(A.2)

Assume that (1) is correct, then we verify indeed that the matrix product $(I - P)(I - P)^{\dagger}$ follows

$$(I - P)\left(\left(I - P + \pi u^{T}\right)^{-1} - \frac{u\pi^{T}}{u^{T}u\pi^{T}\pi}\right) = I - \frac{\pi\pi^{T}}{\pi^{T}\pi}$$
(A.3)

and, similarly, the matrix product $(I - P)^{\dagger} (I - P)$ can be written as

$$\left(\left(I - P + \pi u^T\right)^{-1} - \frac{u\pi^T}{u^T u\pi^T \pi}\right)(I - P) = I - \frac{uu^T}{u^T u}$$
(A.4)

Right multiplying I - P in (A.3) yields

$$(I-P)(I-P)^{\dagger}(I-P) = \left(I - \frac{\pi\pi^{T}}{\pi^{T}\pi}\right)(I-P) = (I-P)$$
(A.5)

Right multiplying $(I - P)^{\dagger}$ in (A.4) results in

$$(I - P)^{\dagger} (I - P) (I - P)^{\dagger} = \left(I - \frac{uu^{T}}{u^{T}u}\right) \left(\left(I - P + \pi u^{T}\right)^{-1} - \frac{u\pi^{T}}{u^{T}u\pi^{T}\pi}\right)$$

= $(I - P)^{\dagger}$ (A.6)

Since matrices $(I - P)(I - P)^{\dagger}$ and $(I - P)^{\dagger}(I - P)$ are symmetric matrices, together with (A.5) and (A.6), we establish Lemma 2.

Appendix B. Proof of Lemma 3

Proof. Let x_k be the eigenvector belonging to the eigenvalue μ_k of the Laplacian Q. The vector $\frac{u}{\sqrt{N}}$ is an eigenvector of Q belonging to the eigenvalue $\mu_N = 0$. The Laplacian matrix can be written as $Q = \sum_{k=1}^{N} \mu_k x_k x_k^T$ and the matrix product QQ^{\dagger} follows

$$QQ^{\dagger} = \sum_{k=1}^{N} \mu_k x_k x_k^T \sum_{m=1}^{N-1} \frac{1}{\mu_m} x_m x_m^T = I - \frac{1}{N} J$$

where matrix $J = uu^T$ is the $N \times N$ all-one matrix. Left multiplying Δ^{-1} yields

$$\Delta^{-1}QQ^{\dagger} = \Delta^{-1} - \frac{\Delta^{-1}u}{N}u^{T}$$

.

The Moore-Penrose pseudo-inverse [22] for the sum of matrices $(A + mn^T)^{\dagger}$ is

$$\left(A + mn^{T}\right)^{\dagger} = A^{\dagger} - kk^{\dagger}A^{\dagger} - A^{\dagger}h^{\dagger}h + \left(k^{\dagger}A^{\dagger}h^{\dagger}\right)kh$$
(B.1)

where $k = A^{\dagger}m$ and $h = n^{T}A^{\dagger}$. Let $A = \Delta^{-1}$, $m = -\frac{\Delta^{-1}u}{N}$ and $n^{T} = u^{T}$, so that $k = \frac{-u}{N}$ and $h = d^{T}$. With $k^{\dagger} = \frac{u^{T}}{N^{2}}$ and $h^{\dagger} = \frac{d}{d^{T}d}$. we arrive at

$$\left(\Delta^{-1} - \frac{\Delta^{-1}u}{N}u^{T}\right)' = \Delta - \frac{u}{N}\frac{u^{T}}{N^{2}}\Delta - \frac{\Delta d}{d^{T}d}d^{T} + \left(\frac{u^{T}}{N^{2}}\Delta\frac{d}{d^{T}d}\right)\frac{u}{N}d^{T}$$

Since $-\frac{u}{N}\frac{u^{T}}{N^{2}}\Delta + \left(\frac{u^{T}}{N^{2}}\Delta\frac{d}{d^{T}d}\right)\frac{u}{N}d^{T} = 0$, Lemma 3 is established.

- [1] J. L. Palacios, On the Kirchhoff index of regular graphs, International Journal of Quantum Chemistry 110 (7) (2010) 1307-1309.
- [2] P. Van Mieghem, Graph spectra for complex networks, Cambridge University Press, 2011.
- [3] M. Fiedler, Algebraic connectivity of graphs, Czechoslovak Mathematical Journal 23 (2) (1973) 298-305.
- [4] D. J. Klein, M. Randić, Resistance distance, Journal of mathematical chemistry 12 (1) (1993) 81–95.
- [5] I. Gutman, W. Xiao, Generalized inverse of the Laplacian matrix and some applications, Bulletin: Classe des sciences mathématiques et natturalles 129 (29) (2004) 15-23.
- [6] P. Van Mieghem, K. Devriendt, H. Cetinay, Pseudo-inverse of the Laplacian and best spreader node in a network, Delft University of Technology, under submission, (2017).
- [7] G. Ranjan, Z.-L. Zhang, Geometry of complex networks and topological centrality, Physica A: Statistical Mechanics and its Applications 392 (17) (2013) 3833 - 3845.
- J. L. Palacios, J. M. Renom, Bounds for the Kirchhoff index of regular graphs via the spectra of their random walks, [8] International Journal of Quantum Chemistry 110 (9) (2010) 1637-1641.
- [9] X. Gao, Y. Luo, W. Liu, Resistance distances and the Kirchhoff index in Cayley graphs, Discrete Applied Mathematics 159 (17) (2011) 2050-2057.
- [10] H. Zhang, Y. Yang, Resistance distance and Kirchhoff index in circulant graphs, International journal of quantum chemistry 107 (2) (2007) 330-339.
- [11] W. Ellens, F. M. Spieksma, P. Van Mieghem, A. Jamakovic, R. E. Kooij, Effective graph resistance, Linear algebra and its applications 435 (10) (2011) 2491-2506.
- [12] X. Wang, E. Pournaras, R. E. Kooij, P. Van Mieghem, Improving robustness of complex networks via the effective graph resistance, The European Physical Journal B 87 (9) (2014) 221.
- [13] X. Wang, Y. Koç, R. E. Kooij, P. Van Mieghem, A network approach for power grid robustness against cascading failures, in: Reliable Networks Design and Modeling (RNDM), 2015 7th International Workshop on, IEEE, 2015, pp. 208–214.
- [14] J. G. Kemeny, Generalization of a fundamental matrix, Linear Algebra and its Applications 38 (1981) 193-206.
- [15] C. M. Grinstead, J. L. Snell, Introduction to Probability 2nd Edition, 2003.
- [16] M. Levene, G. Loizou, Kemeny's constant and the random surfer, The American mathematical monthly 109 (8) (2002) 741-745.
- [17] S. Kirkland, Fastest expected time to mixing for a Markov chain on a directed graph, Linear Algebra and its Applications 433 (11-12) (2010) 1988-1996.
- [18] S. Kirkland, Z. Zeng, Kemeny's constant and an analogue of Braess' paradox for trees, Electronic Journal of Linear Algebra 31 (1) (2016) 444-464.
- [19] J. J. Hunter, The role of Kemeny's constant in properties of Markov chains, Communications in Statistics-Theory and Methods 43 (7) (2014) 1309–1321.
- [20] F. Fouss, A. Pirotte, J.-M. Renders, M. Saerens, Random-walk computation of similarities between nodes of a graph with application to collaborative recommendation, IEEE Transactions on knowledge and data engineering 19 (3) (2007) 355-369.
- [21] Z. Zhang, B. Wu, H. Zhang, S. Zhou, J. Guan, Z. Wang, Determining global mean-first-passage time of random walks on Vicsek fractals using eigenvalues of Laplacian matrices, Physical Review E 81 (3) (2010) 031118.
- [22] S. L. Campbell, C. D. Meyer, Generalized inverses of linear transformations, SIAM, 2009.
- [23] J. L. Palacios, J. M. Renom, Broder and Karlin's formula for hitting times and the Kirchhoff Index, International Journal of Ouantum Chemistry 111 (1) (2011) 35-39.
- [24] H. Chen, F. Zhang, Resistance distance and the normalized Laplacian spectrum, Discrete Applied Mathematics 155 (5) (2007) 654-661.

- [25] I. Ž. Milovanović, E. I, Milovanović, On some lower bounds of the Kirchhoff index, MATCH Commun. Math. Comput. Chem 78 (2017) 169–180.
- [26] Y. Yang, Some bounds for the Kirchhoff index of graphs, in: Abstract and Applied Analysis, Vol. 2014, Hindawi Publishing Corporation, 2014.
- [27] I. Ž. Milovanović, E. I. Milovanović, E. Glogić, Lower bounds of the Kirchhoff and degree Kirchhoff indices, Scientific Publications of the State University of Novi Pazar Series A: Applied Mathematics, Informatics and mechanics 7 (1) (2015) 25–31.
- [28] P. Van Mieghem, Performance analysis of complex networks and systems, Cambridge University Press, 2014.
- [29] J. L. Palacios, A new lower bound for the multiplicative degree-Kirchhoff index, MATCH Commun. Math. Comput. Chem 76 (1) (2016) 251–254.
- [30] P. Erdős, A. Rényi, On random graphs I., Publ. Math. Debrecen 6 (1959) 290–297.
- [31] A.-L. Barabási, R. Albert, Emergence of scaling in random networks, science 286 (5439) (1999) 509-512.
- [32] D. J. Watts, S. H. Strogatz, Collective dynamics of 'small-world' networks, Nature 393 (6684) (1998) 440-442.