Kirchhoffian indices for weighted digraphs

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Abstract

The resistance indices, namely the Kirchhoff index and its generalisations, have undergone intense critical scrutiny in recent years. Based on random walks, we derive three Kirchhoffian indices for strongly connected and weighted digraphs. These indices are expressed in terms of (i) hitting times and (ii) the trace and eigenvalues of suitable matrices associated to the graph, namely the asymmetric Laplacian, the diagonally scaled Laplacian and their Moore-Penrose inverses. The appropriateness of the generalised Kirchhoff index as a measure of network robustness is discussed, providing an alternative interpretation which is supported by an empirical application to the World Trade Network.

Keywords: Kirchhoff index; Random walk on graphs; Weighted digraphs; Moore-Penrose inverse

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1. Introduction

On a simple connected graph G = (V, E), it is possible to define a multitude of descriptors aimed at characterising and quantifying its structural properties, which are preserved by a graph isomorphism. These descriptors, often referred to as graph invariants or topological indices, are particularly useful in practical applications. Amongst these descriptors, the resistive indices — namely the Kirchhoff index and its generalisations, such as the multiplicative and the additive Kirchhoff indices — have received considerable attention in e.g. chemical applications, because they have proven to be useful in discriminating among chemical molecules (=undirected graphs), with their atoms (=vertices) and bonds (=edges), according to their cyclicity (see [1–8]).

A natural extension motivated by the node/edge structure of real networks is to think of Kirchhoff-type descriptors defined on strongly connected and weighted digraphs. In this context, there are ways to define effective resistances between nodes so as to provide a possible generalisation of the Kirchhoff index (e.g.[9],[10]), even though it may be argued that the physical interpretation of these generalised effective resistances remains elusive (for instance: these effective resistances do not satisfy the triangular inequality).

Following the probabilistic approach to the Kirchhoff index based on the random walk on a graph [1], this paper aims at providing different expressions of the Kirchhoff-type descriptors in terms of (i) hitting and commute times and (ii) the trace and eigenvalues of suitable matrices associated to the graph, namely the asymmetric Laplacian, the diagonally scaled Laplacian and their Moore-Penrose inverses. Moreover, interesting relationships interlacing these indices are derived.

It is worth pointing out that the Kirchhoff index for undirected and weighted graphs gives a measure of the *robustness* of a network, i.e. the capacity of a network to maintain functionality — through back-up paths — in the presence of node failure. In particular, it is important to stress the monotonicity of the Kirchhoff index within this context. Indeed, adding an edge, or increasing the weight of an edge, yields a graph with a smaller total effective resistance, i.e. a smaller Kirchhoff index (see Theorem 2.7 in [11]).

On the other hand, the additive and multiplicative Kirchhoff indices are not monotonic even in the case of undirected graphs. Thus, the minimum requirement for an index to be a suitable robustness measure is not satisfied.

Following the presentation of our analytical results, we show that, in the case of directed networks, the Kirchhoff index can no longer correspond to a robustness measure (as defined above), and we suggest an alternative interpretation within the framework of random walks on graphs. Moreover, we further argue about the usefulness of the Kirchhoff-type descriptor proposed with an empirical illustrative application to the World Trade Network.

2. Notation and preliminaries

We quickly recall some standard definitions and results about graph theory and random walks on graphs; for more details the reader is referred to [12], [13] and [14].

A graph G = (V, E) is a pair of sets (V, E), where V is the set of n vertices and E is the set of m pairs of vertices of V. Let us denote with |V| and |E| the cardinality of the sets V and E, respectively. An undirected graph is a graph in which $(j, i) \in E$ whenever $(i, j) \in E$, whereas a directed graph (digraph, hereinafter) is a graph in which each edge (arc) is an ordered pair (i, j) of vertices. Moreover, a weight w_{ij} is possibly associated to each edge (i, j), in this case we will have a weighted (or valued) graph.

By *simple graph* we refer to an unweighted, undirected graph containing no self-loops or multiple edges [12].

A non-negative n-square matrix \mathbf{A} , representing the adjacency relationships between vertices of G, is associated to the graph (the adjacency matrix); the off-diagonal elements a_{ij} of \mathbf{A} are equal to 1 if vertices i and j are adjacent, 0 otherwise; if the graph has self-loops the corresponding diagonal elements of \mathbf{A} are equal to 1. If G = (V, E) is a digraph, its adjacency matrix is in general asymmetric. In the sequel we denote by $\mathbf{W} = [w_{ij}]$ the weighted adjacency matrix of a weighted digraph G.

For an undirected graph G, the degree d_i of vertex i ($i = 1, \dots, n$) is the number of edges incident to it. In a digraph the in-degree $d_i^{(in)}$ of a vertex i, is the number of arcs directed from other vertices to i and the out-degree $d_i^{(out)}$ of a vertex i is the number of arcs directed

from i to other vertices. For weighted graphs we have $d_i^{(out)} = \sum_{j=1}^n w_{ij}$ and $d_i^{(in)} = \sum_{j=1}^n w_{ji}$, for i = 1, ..., n. In general $d_i^{(out)} \neq d_i^{(in)}$ but

$$\sum_{i=1}^{n} d_i^{(out)} = \sum_{i=1}^{n} d_i^{(in)} = \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij}$$

and we refer to this quantity as the volume Vol(G) of the weighted digraph G. For simple graphs, we have Vol(G) = 2|E|.

In the sequel we deal with the general case of weighted digraphs and we focus on outdegrees underlining that all the results can be carried out also for in-degrees taking the transpose of the weighted adjacency matrix.

Let us assume that every vertex has at least one out-going edge which can include selfloops, i.e $d_i^{(out)} \neq 0$ for every i. In this case, the matrix $\mathbf{D} = \operatorname{diag}(d_i^{(out)})$ is non singular and we can define $\mathbf{P} = \mathbf{D}^{-1}\mathbf{W}$ as the transition probability matrix of the Markov chain associated with a random walk on G. Thus $p_{ij} = w_{ij}/d_i^{(out)}$ is the probability of transiting from vertex i to vertex j and it is different from zero when $(i, j) \in E$.

If the graph G is strongly connected, i.e. for any pair of vertices there is a directed path leading from one vertex to the other, \mathbf{P} is irreducible and the associated Markov chain is said to be ergodic. By the Perron-Frobenius theorem, there exists a unique positive vector of stationary probabilities $\boldsymbol{\pi} = [\pi_j]$ such that $\boldsymbol{\pi}^T \mathbf{P} = \boldsymbol{\pi}^T$ and $\boldsymbol{\pi}^T \mathbf{e} = 1$, where \mathbf{e} denotes the $n \times 1$ vector consisting of all ones.

Recall that for any ergodic chain the matrix $(\mathbf{I} - \mathbf{P} + \mathbf{e} \boldsymbol{\pi}^T)$ is non singular and its inverse \mathbf{Z} is known as the fundamental matrix of the chain ([13], [14]). In case of a regular chain, i.e. a chain for which \mathbf{P} is primitive, we have

$$\mathbf{Z} = \sum_{k=0}^{\infty} (\mathbf{P} - \mathbf{e}\boldsymbol{\pi}^{T})^{k} = \mathbf{I} + \sum_{k=1}^{\infty} (\mathbf{P}^{k} - \mathbf{e}\boldsymbol{\pi}^{T})$$
 (1)

Another useful matrix associated to the graph G is the (ordinary) asymmetric Laplacian matrix $\mathbf{L} = \mathbf{\Pi}(\mathbf{I} - \mathbf{P})$, where $\mathbf{\Pi} = \operatorname{diag}(\pi_i)$. It is well known that $\operatorname{rank}(\mathbf{L}) = n - 1$, and $\operatorname{Le} = \mathbf{L}^T \mathbf{e} = \mathbf{0}$.

Moreover, $\mathbf{L} + \boldsymbol{\pi} \boldsymbol{\pi}^T$ is non singular, and its inverse $\widetilde{\mathbf{Z}}$ is related to the fundamental matrix \mathbf{Z} by the formula $\widetilde{\mathbf{Z}} = \mathbf{Z} \mathbf{\Pi}^{-1}$.

If we denote by M the Moore-Penrose inverse of L, it can be proved that

$$\mathbf{M} = (\mathbf{I} - \mathbf{E}/n)\widetilde{\mathbf{Z}}(\mathbf{I} - \mathbf{E}/n)$$

where $\mathbf{E} = \mathbf{e}\mathbf{e}^T$ (see, for instance, [15], Lemma 14). Note that $\mathbf{M}\mathbf{e} = \mathbf{e}^T\mathbf{M} = \mathbf{0}$.

The matrices \mathbf{M} and \mathbf{Z} play a central role in defining the expected hitting time. The hitting time T_j is the number of transitions needed by a random walker on G to reach j for the first time and its expected value, also known as mean first passage time (MFPT, hereinafter), when she/he starts at i, is denoted by H(i,j). By convention $H(i,i) = 0, \forall i$ while for $i \neq j$ it is well known that

$$H(i,j) = \frac{z_{jj} - z_{ij}}{\pi_j}. (2)$$

We recall from [15], Theorem 15, the following expression to obtain the expected hitting time in terms of the Moore-Penrose inverse M of the Laplacian matrix L:

$$H(i,j) = m_{jj} - m_{ij} + \sum_{k=1}^{n} (m_{ik} - m_{jk}) \pi_k.$$

In contrast with the expected hitting time H(i,j), which is in general not symmetric, the commute time, defined as

$$C(i,j) = C(j,i) = H(i,j) + H(j,i) = m_{jj} + m_{ii} - m_{ij} - m_{ji}$$
(3)

is a symmetric measure.

In what follows, we will be interested in partial sums of hitting times. The Random Target Lemma ([13],[16]), states that

$$\sum_{i=1}^{n} \pi_j H(i,j)$$

is a constant K not depending on i, usually called Kemeny's constant. It can be expressed in terms of the eigenvalues $\nu_i \neq \nu_1 = 1$ of the matrix \mathbf{P} as

$$K = \sum_{i=2}^{n} \frac{1}{1 - \nu_i}.$$
 (4)

3. Kirchhoffian descriptors: Analytical properties

In this section we present a generalisation of the Kirchhoff-type indices, namely the Kirchhoff index, the multiplicative and the additive Kirchhoff indices, for strongly connected, directed and weighted (DW- hereinafter) graphs, both in terms of suitable Laplacian matrices and their eigenvalues.

3.1. DW-Kirchhoff index

For a simple connected graph G = (V, E), the Kirchhoff index was defined by Klein and Randić in [2] as

$$R(G) = \sum_{i=1}^{n} \sum_{j=i+1}^{n} R_{ij},$$

where R_{ij} is the effective resistance as defined by Ohm's law when a battery is placed between i and j so that the current entering at i is 1 and the voltage at j is 0. An algebraic approach to R(G) (see [3] and [4]) yielded the representation

$$R(G) = n \sum_{i=1}^{n-1} \frac{1}{\lambda_i},$$
 (5)

where the λ_i 's are the non-zero eigenvalues of the Laplacian $\mathcal{L} = \Delta - \mathbf{A}$, with $\Delta = \operatorname{diag}(d_i)$ and \mathbf{A} being the adjacency matrix of G. There is also an obvious connection between R(G) and expected hitting times that was noticed first in [1]:

$$R(G) = \frac{1}{2|E|} \sum_{i,j=1}^{n} H(i,j).$$

This probabilistic definition of R(G) allows us to define for strongly connected, weighted digraphs the DW-Kirchhoff index as follows:

$$S(G) = \frac{1}{\text{Vol}(G)} \sum_{i,j=1}^{n} H(i,j).$$
 (6)

In what follows we derive two different equivalent formulas for the DW-Kirchhoff index. The first one gives S(G) in terms of the trace of \mathbf{M} , while the latter generalises formula (5). **Proposition 1.** For any strongly connected, weighted digraph G, we have

$$S(G) = \frac{n}{\text{Vol}(G)} \operatorname{Trace}(\mathbf{M}); \tag{7}$$

or equivalently,

$$S(G) = \frac{n}{\text{Vol}(G)} \sum_{i=1}^{n-1} \frac{1}{\mu_i},$$
(8)

where the μ_i 's are the non-zero eigenvalues of the asymmetric Laplacian L.

Proof. Formula (7) derives easily from (2) taking into account that $\mathbf{Me} = \mathbf{0}$, while the proof of (8) follows the same line of Corollary 2 of [17].

First of all, from the properties of the fundamental matrix **Z**, we get

$$(\mathbf{I} - \mathbf{E}/n) = (\mathbf{L} + \boldsymbol{\pi} \boldsymbol{\pi}^{\mathrm{T}}) \mathbf{Z} \boldsymbol{\Pi}^{-1} (\mathbf{I} - \mathbf{E}/n) = (\mathbf{L} + \mathbf{e} \boldsymbol{\pi}^{\mathrm{T}}) \mathbf{Z} \boldsymbol{\Pi}^{-1} (\mathbf{I} - \mathbf{E}/n).$$

Since $(\mathbf{L} + \mathbf{e}\boldsymbol{\pi}^T)$ is non singular,

$$\mathbf{Z}\mathbf{\Pi}^{-1}(\mathbf{I} - \mathbf{E}/n) = (\mathbf{L} + \mathbf{e}\boldsymbol{\pi}^{T})^{-1}(\mathbf{I} - \mathbf{E}/n)$$

and

$$S(G) = \frac{n}{\text{Vol}(G)} \text{Trace}(\mathbf{U}^{T} (\mathbf{L} + \mathbf{e} \boldsymbol{\pi}^{T})^{-1} (\mathbf{I} - \mathbf{E}/n) \mathbf{U})$$

where **U** is an orthonormal matrix with $\frac{1}{\sqrt{n}}\mathbf{e}$ as its first column. Standard computations on block matrices, show that the trace of the matrix $(\mathbf{U}^T(\mathbf{L} + \mathbf{e}\boldsymbol{\pi}^T)^{-1}(\mathbf{I} - \mathbf{E}/n)\mathbf{U})$ is given by the sum of the non-zero eigenvalues of the asymmetric Laplacian matrix **L**.

Note that even if some of the eigenvalues of the Laplacian matrix \mathbf{L} might be complex, the sum in (8) is real since the complex eigenvalues are always present in conjugate pairs.

3.2. DW-Multiplicative Kirchhoff index

On a simple connected graph G = (V, E), the multiplicative degree-Kirchhoff index, proposed by [7] was defined as

$$R^*(G) = \sum_{i=1}^n \sum_{j=i+1}^n d_i d_j R_{ij},$$
(9)

where d_i is the degree of the vertex i and R_{ij} is the effective resistance between vertices i and j. An algebraic approach to $R^*(G)$ yielded the representation

$$R^*(G) = 2|E| \sum_{i=1}^{n-1} \frac{1}{\lambda_i^*},\tag{10}$$

where the λ_i^* 's are the non-zero eigenvalues of the diagonally-scaled Laplacian $\mathcal{L}^d = \Delta^{1/2} \mathcal{L} \Delta^{-1/2}$ (see [7]), or equivalently $\lambda_i^* = 1 - \nu_i$, where the ν_i 's are the eigenvalues not equal to 1 of the transition probability matrix $\mathbf{P} = \Delta^{-1} \mathbf{A}$ of the random walk on G (see [18]). Also, in terms of expected hitting times, we get

$$R^*(G) = 2|E| \sum_{i,j=1}^n \pi_i \pi_j H(i,j).$$
(11)

where $\pi_i = d_i/2|E|$, for the case of simple graphs.

According to the expression above, we can define the DW-multiplicative $Kirchhoff\ index$ as

$$S^*(G) = \text{Vol}(G) \sum_{i,j=1}^{n} \pi_i \pi_j H(i,j).$$
 (12)

Note that by the Random Target Lemma,

$$S^*(G) = \text{Vol}(G) \sum_{j=1}^n \pi_j H(i, j), \text{ for any } i.$$
 (13)

Thus, up to a multiplicative constant, $S^*(G)$ represents the average of the expected hitting times with weights given by the elements of the stationary distribution vector $\boldsymbol{\pi}$ (see [16]).

In the next proposition we give alternative expressions of the DW-multiplicative Kirchhoff index.

Proposition 2. For any strongly connected, weighted digraph

$$S^*(G) = \operatorname{Vol}(G) \operatorname{Trace}(\mathbf{M}^d)$$

where \mathbf{M}^d is the Moore-Penrose inverse of the diagonally scaled asymmetric Laplacian $\mathbf{L}^d = \mathbf{\Pi}^{1/2}\mathbf{L}\mathbf{\Pi}^{-1/2}$, or, equivalently,

$$S^*(G) = \operatorname{Vol}(G) \operatorname{Trace}(\mathbf{\Pi} \mathbf{M}) - \boldsymbol{\pi}^T \mathbf{M} \boldsymbol{\pi}.$$
 (14)

Moreover,

$$S^*(G) = \text{Vol}(G) \sum_{i=2}^{n} \frac{1}{1 - \nu_i},$$
(15)

where the ν_i 's are the eigenvalues (not equal to 1) of the transition probability matrix \mathbf{P} .

Proof. Formulas (13) and (2) give

$$S^*(G) = \operatorname{Vol}(G)(\operatorname{Trace}(\mathbf{Z}) - 1).$$

Taking into account Definition 9 and Lemma 14 in [15], setting $\sqrt{\pi} = (\sqrt{\pi_1}, \cdots, \sqrt{\pi_n})^T$ and $\mathbf{Z}^d = \mathbf{\Pi}^{1/2} \widetilde{\mathbf{Z}} \mathbf{\Pi}^{1/2}$, we get

$$S^*(G) = \operatorname{Vol}(G) \ (\operatorname{Trace}(\widetilde{\mathbf{Z}}\boldsymbol{\Pi}) - 1) = \operatorname{Vol}(G) \ (\operatorname{Trace}(\boldsymbol{\Pi}^{1/2}\widetilde{\mathbf{Z}}\boldsymbol{\Pi}^{1/2}) - 1) =$$

$$= \operatorname{Vol}(G) \ (\operatorname{Trace}(\mathbf{Z}^d) - \operatorname{Trace}(\sqrt{\pi}\sqrt{\pi}^T)) =$$

$$= \operatorname{Vol}(G) \ \operatorname{Trace}(\mathbf{M}^d).$$

Now, by the calculus rules of the Moore-Penrose inverse,

$$\mathbf{M}^d = (\mathbf{I} - \sqrt{\pi}\sqrt{\pi}^T)\mathbf{\Pi}^{1/2}\mathbf{M}\mathbf{\Pi}^{1/2}(\mathbf{I} - \sqrt{\pi}\sqrt{\pi}^T),$$

by the idempotent property of $(\mathbf{I} - \sqrt{\pi}\sqrt{\pi}^T)$, and the equality $\mathbf{\Pi}^{1/2}\sqrt{\pi} = \pi$ we get

$$\begin{split} \operatorname{Trace}(\mathbf{M}^d) &= \operatorname{Trace}(\mathbf{\Pi}^{1/2}\mathbf{M}\mathbf{\Pi}^{1/2}(\mathbf{I} - \sqrt{\boldsymbol{\pi}}\sqrt{\boldsymbol{\pi}}^{\, T})) = \\ &= \operatorname{Trace}(\mathbf{\Pi}^{1/2}\mathbf{M}\mathbf{\Pi}^{1/2}) - \operatorname{Trace}(\mathbf{\Pi}^{1/2}\mathbf{M}\mathbf{\Pi}^{1/2}\sqrt{\boldsymbol{\pi}}\sqrt{\boldsymbol{\pi}}^{\, T}) = \\ &= \operatorname{Trace}(\mathbf{\Pi}\mathbf{M}) - \operatorname{Trace}(\boldsymbol{\pi}^{\, T}\mathbf{M}\boldsymbol{\pi}) = \operatorname{Trace}(\mathbf{\Pi}\mathbf{M}) - \boldsymbol{\pi}^{\, T}\mathbf{M}\boldsymbol{\pi} \end{split}$$

Therefore expression (14) follows. Finally, the third expression is a direct consequence of (4).

3.3. DW-Additive Kirchhoff index

On a simple connected graph G = (V, E), the additive degree-Kirchhoff index, proposed by [8] was defined as

$$R^{+}(G) = \sum_{i=1}^{n} \sum_{j=i+1}^{n} (d_i + d_j) R_{ij},$$
(16)

where d_i is the degree of the vertex i and R_{ij} is the effective resistance between vertices i and j. By the random walk approach, it is known that $2|E|R_{ij} = H(i,j) + H(j,i) = C(i,j)$ (see for instance, [17]). Thus recalling that $d_i = 2\pi_i |E|$, we can rewrite (16) as

$$R^{+}(G) = \frac{1}{2} \sum_{i,j=1}^{n} (\pi_i + \pi_j) C(i,j)$$

and this definition makes sense in any strongly connected, weighted digraph G. Thus we introduce the directed weighted additive Kirchhoff index (DW-additive Kirchhoff index, for brevity) as a weighted average of the commute times between each pair of nodes, with weights given by $(\pi_i + \pi_j)/2$:

$$S^{+}(G) = \frac{1}{2} \sum_{i,j=1}^{n} (\pi_i + \pi_j) C(i,j).$$
 (17)

In the next Proposition we put in evidence an interesting link between the DW-additive Kirchhoff index and the DW-Kirchhoff index, already noted by Yang and Klein for unweighted undirected graphs (see Theorem 3 in [19]), and, in addition, we give also a link with the DW-multiplicative Kirchhoff index.

Proposition 3. For any strongly connected, weighted digraph

$$S^{+}(G) = \frac{\operatorname{Vol}(G)}{n} S(G) + n \operatorname{Trace}(\mathbf{\Pi}\mathbf{M}). \tag{18}$$

Moreover,

$$S^{+}(G) = \frac{\operatorname{Vol}(G)}{n} S(G) + \frac{n}{\operatorname{Vol}(G)} S^{*}(G) + n \,\boldsymbol{\pi}^{T} \mathbf{M} \boldsymbol{\pi}$$
(19)

Proof. Equation (18) follows from (3) and (7). To prove (19) we relate the last summand in (18) with the DW-multiplicative Kirchhoff index. Indeed, by (14),

$$\operatorname{Trace}(\mathbf{\Pi}\mathbf{M}) = \frac{1}{\operatorname{Vol}(G)} S^*(G) + \boldsymbol{\pi}^{\mathrm{T}} \mathbf{M} \boldsymbol{\pi}$$

and the assertion follows.

In the next Proposition we give an expression of the DW-additive Kirchhoff index in terms of the sum of eigenvalues of suitable matrices (for the case concerning simple graphs, see [20]).

Proposition 4. For any strongly connected, weighted digraph

$$S^{+}(G) = \sum_{i=1}^{n} \frac{1}{\alpha_i} + n \sum_{i=2}^{n} \frac{1}{1 - \nu_i} - n$$
 (20)

where the $\alpha_i s$ are the eigenvalues of the modified laplacian matrix $\mathbf{L} + \boldsymbol{\pi} \boldsymbol{\pi}^T$ and the $\nu_i' s$ the eigenvalues (not equal to 1) of the transition probability matrix \mathbf{P} .

Proof. Starting by (19), let us consider the term

$$\frac{\operatorname{Vol}(G)}{n}S(G) + n\,\boldsymbol{\pi}^{\scriptscriptstyle T}\mathbf{M}\boldsymbol{\pi} = \operatorname{Trace}((\mathbf{I} + n\boldsymbol{\pi}\boldsymbol{\pi}^{\scriptscriptstyle T})\mathbf{M})$$

Inserting the expression of $\mathbf{M} = (\mathbf{I} - \mathbf{E}/n)\tilde{\mathbf{Z}}(\mathbf{I} - \mathbf{E}/n)$ and taking into account the relations $\tilde{\mathbf{Z}} = \mathbf{Z}\boldsymbol{\Pi}^{-1}$ and $\boldsymbol{\pi}^T\mathbf{Z} = \boldsymbol{\pi}^T$, after some algebra we get

$$\operatorname{Trace}((\mathbf{I} + n\boldsymbol{\pi}\boldsymbol{\pi}^T)\mathbf{M}) = \operatorname{Trace}(\tilde{\mathbf{Z}}) - n.$$

The assertion follows by the definition of the matrix $\tilde{\mathbf{Z}} = (\mathbf{L} + \boldsymbol{\pi}\boldsymbol{\pi}^T)^{-1}$ and by Proposition 2.

As a summarising device, we report in Table 1 below alternative expressions for the Kirchhoff-type descriptors derived so far. Recall that the μ_i 's are the non-zero eigenvalues of the asymmetric Laplacian \mathbf{L} , the ν_i 's are the eigenvalues (not equal to 1) of the transition probability matrix \mathbf{P} while the α_i s are the eigenvalues of the modified Laplacian matrix $(\mathbf{L} + \boldsymbol{\pi} \boldsymbol{\pi}^T)$.

Table 1: Alternative expressions of Kirchhoff-type descriptors

Index	H(i,j) or $C(i,j)$	Moore-Penrose	Eigenvalues
S(G)	$\frac{1}{\operatorname{Vol}(G)} \sum_{i,j=1}^{n} H(i,j)$	$\frac{n}{\operatorname{Vol}(G)}\operatorname{Trace}(\mathbf{M})$	$\frac{n}{\operatorname{Vol}(G)} \sum_{i=1}^{n-1} \frac{1}{\mu_i}$
$S^*(G)$	$\operatorname{Vol}(G) \sum_{j=1}^{n} \pi_{j} H(i, j)$	$\operatorname{Vol}(G)\operatorname{Trace}(\mathbf{M}^d)$	$\operatorname{Vol}(G) \sum_{i=2}^{n} \frac{1}{1 - \nu_i}$
$S^+(G)$	$\frac{1}{2}\sum_{i,j=1}^{n}(\pi_i+\pi_j)C(i,j)$	$\operatorname{Trace}(\mathbf{M}) + n\operatorname{Trace}(\mathbf{\Pi}\mathbf{M})$	$\sum_{i=1}^{n} \frac{1}{\alpha_i} + n \sum_{i=2}^{n} \frac{1}{1 - \nu_i} - n$

4. Kirchhoffian descriptors: discussion and empirical application

The Kirchhoff index for the case of weighted, undirected graphs has been advocated as a suitable measure of network robustness [21]. The fact that the index decreases monotonically when an edge is added (or the weight of an existing link increased) allows us to unambiguously associate a decrease in total effective resistance to a higher network robustness. This monotonicity property, however, does not automatically extend to the additive and multiplicative indices or to the DW-Kirchhoff index introduced in section 3.⁵

In this section we discuss the monotonicity property for (i) the multiplicative and additive Kirchhoff indices (for undirected graphs) and (ii) the DW-Kirchhoff index, providing an alternative interpretation for S(G) as a closeness centrality index. Such an interpretation is illustrated with an empirical application to the World Trade Network, comparing also S(G) with $S^*(G)$ and $S^+(G)$, within this context.

4.1. Discussion: Undirected graphs

The following example shows that the monotonicity property does not hold for the multiplicative and additive Kirchhoff indices, already within the context of undirected graphs. Figure 1 reports first the adjacency matrix of graph G_1 . We then represent graphs G_2 and G_3 : G_2 is identical to G_1 with an added link between nodes 1 and 5, whereas G_3 is identical to G_2 with a further edge between nodes 1 and 6.

Given the added paths between vertices, we would expect the additive and multiplicative Kirchhoff indices to decrease. However, as can be seen from Table 2, while total effective resistance R(G) decreases as links are added, $R^*(G)$ and $R^+(G)$ do not follow a monotonic trend: both indices *increase* (when considering the change between G_1 and G_2) and then decrease (when considering the change between G_2 and G_3).

Thus, already in the undirected case the monotonicity property only holds for the Kirchhoff index and not for the additive and multiplicative variants. Taking this result into account, we concentrate on the DW-Kirchhoff index in what follows.

⁵We wish to thank an anonymous referee for his insightful comment, directing our attention to this issue.

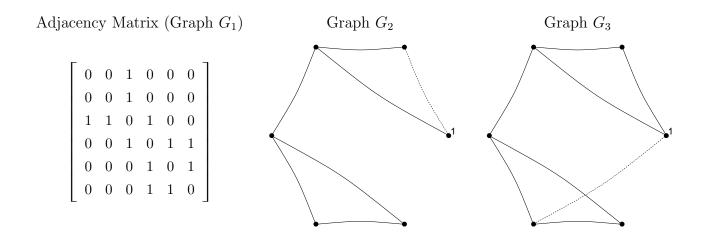


Figure 1: Behaviour of R(G), $R^*(G)$ and $R^+(G)$. Adjacency matrix of G_1 ; G_2 is equal to G_1 with an additional edge between nodes 1 and 2, whereas G_3 adds a further edge to G_2 between nodes 1 and 5. Nodes in the adjacency matrix go from 1 to 6, nodes in graphs are numbered counter-clockwise, starting from node 1 (labelled); added edge with a *dashed* line type.

Table 2: Behaviour of R(G), $R^*(G)$ and $R^+(G)$

	G_1	G_2	G_3
R(G)	25	21	12.7
$R^*(G)$	81	107.6	85.6
$R^+(G)$	92	95.3	66.1

4.2. Discussion: Directed, weighted graphs

In the examples below we analyse three possible outcomes for the behaviour of S(G) when an edge is added with progressively higher weight: S(G) is (i) monotonically increasing, (ii) conditional upon the weight of the new link or (iii) monotonically decreasing. Figure 2 depicts three strongly connected graphs G_1 , G_2 and G_3 , one corresponding to each of the cases (i)-(iii).

To grasp the behaviour of the relevant magnitudes of each example in some detail, Table 3 reports (for varying link weights) S(G) and its components, according to (6), noting that it may be written as:

$$S(G) = \frac{1}{\text{Vol}(G)} \sum_{i,j=1}^{n} H(i,j) = \frac{n}{\text{Vol}(G)} \sum_{j=1}^{n} \bar{H}(j), \text{ where } \bar{H}(j) = (1/n) \sum_{i=1}^{n} H(i,j)$$

i.e. $\bar{H}(j)$ is the average hitting time to reach node j, averaging over possible source nodes in the network.

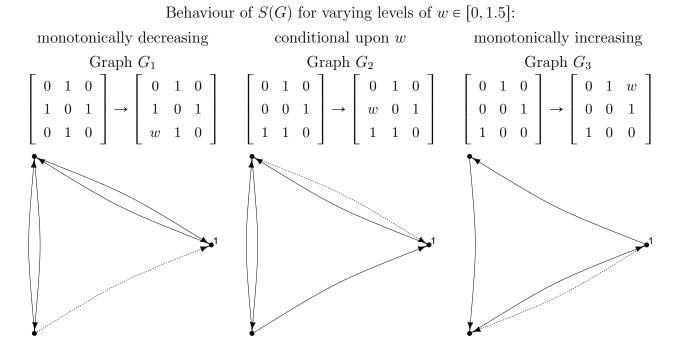


Figure 2: Behaviour of S(G) for varying levels of an additional link $w \in [0, 1.5]$. Graphs and adjacency matrices of G_1 , G_2 and G_3 . Nodes in the adjacency matrix go from 1 to 3, nodes in graphs are numbered counter-clockwise, starting from node 1 (labelled); added edge with a *dashed* line type.

Table 3: Behaviour of S(G)

	F4.7	[0]	[0]	Γ 4 7		[6]	[7]	[0]	[0]	[40]	F4.4.7	[40]	
(column #)	[1]	[2]	[3]	[4]	[5]	[6]	[7]	[8]	[9]	[10]	[11]	[12]	
Graph		C	r_1			G_2				G_3			
New Link	$3 \rightarrow 1$					$2 \rightarrow 1$				$1 \rightarrow 3$			
Link Weight w	0.00	0.50	1.00	1.50	0.00	0.50	1.00	1.50	0.00	0.50	1.00	1.50	
S(G)	4.00	3.13	2.70	2.40	3.13	2.72	2.70	2.75	3.00	3.50	4.00	4.50	
Vol(G)	4.00	4.50	5.00	5.50	4.00	4.50	5.00	5.50	3.00	3.05	3.13	3.20	
$\sum_{i,j} H(i,j)$	16.00	14.08	13.50	13.23	12.50	12.25	13.50	15.13	9.00	10.67	12.50	14.40	
$ar{H}(1)$	2.33	1.58	1.33	1.21	2.33	1.58	1.33	1.21	1.00	1.00	1.00	1.00	
$ar{H}(2)$	0.67	0.78	0.83	0.87	0.83	0.83	0.83	0.83	1.00	1.67	2.33	3.00	
$\bar{H}(3)$	2.33	2.33	2.33	2.33	1.00	1.67	2.33	3.00	1.00	0.89	0.83	0.80	

In graph G_1 , nodes 1 and 3 are originally only connected through node 2, and setting up

an edge from 3 to 1 decreases S(G), irrespective of the link weight w. In graph G_2 , adding a link from node 2 to 1 makes it possible to reach the latter without necessarily passing by node 3. In this case, there is a switchover in the behaviour of S(G) (first decreases and then increases) as w varies at some point between w = 0.5 and w = 1.5. Finally, an edge from node 1 to 3 is added in the cycle graph G_3 , and S(G) increases, irrespective of the link weight w.

Thus, there is no unambiguous behaviour for the DW-Kirchhoff index S(G) when adding an edge or increasing the weight of an existing link. In order to understand the determinants of this outcome, we focus on the general pattern of behaviour of average hitting times $\bar{H}(j)$.

In all three graphs, the average hitting time of the source node in the new link remains unaltered (possible paths to be reached as a target have not changed), whereas the average mean first passage time of the target node in the new link decreases (possible paths to be reached increase). Interestingly, the average hitting time of the remaining node(s) increases. Hence, the uneven behaviour in $\bar{H}(j)$ determines the outcome observed: when the decrease in the target node is higher than the increase in other nodes, the DW-Kirchhoff index decreases. Therefore, S(G) as formulated in (6) does not behave monotonically when a new edge is added, hindering its use as a measure of network robustness for the case of directed graphs.

4.3. Random Walk on Graphs and Kirchhoffian descriptors in the World Trade Network

A meaningful alternative interpretation of the DW-Kirchhoff index consists in considering the mean of H(i,j) from all source nodes i to a given target node j — denoted above by $\overline{H}(j)$ — as providing a local measure of closeness centrality (labelled random-walk centrality in [22]):

$$C_{rw}(j) = \frac{1}{\overline{H}(j)}$$

conveying the notion of how immediately, on average, every node reaches node j.

⁶Examples involving networks with a higher number of nodes confirm this pattern.

Under this light, $S(G)^{-1}$ can be interpreted as a measure of average closeness centrality across nodes:

$$S(G)^{-1} = \frac{\text{Vol}(G)}{\sum_{i,j=1}^{n} H(i,j)} = \frac{\text{Vol}(G)}{n^2} \times \left(\frac{n}{\sum_{j=1}^{n} C_{rw}(j)^{-1}}\right)$$
(21)

i.e. an *harmonic* average (up to a multiplicative term) of random walk centrality scores for each target node j.⁷

Interpreting S(G) as a global measure of closeness centrality in a context of weighted, directed graphs becomes useful when available indicators require to transform the original graph into an undirected network, discarding crucial information as regards the direction of flows. One such example within the field of economic networks is the World Trade Network (WTN, hereinafter) (see, e.g. [24, ch. 2]).

The WTN is the graph representation of the recorded set of trade transactions in goods and services between countries. Nodes represent trading partners and the outgoing and incoming links stand for export and import flows, respectively. In its original form, it can be interpreted as a weighted (by the flow value in USD), directed (asymmetric import/export links) graph. However, applications usually transform original data to obtain either a binary and/or symmetric network, in order to fit the indicators readily available [25, 26].

Our aim is to show that, by recourse to our DW-Kirchhoff index S(G) it is possible to depict the evolution of global random walk closeness centrality of the WTN more accurately than the picture portrayed by indicators computed on undirected and/or unweighted data.

Moreover, the standard formulation of the concept of random walk centrality from an operational perspective (e.g. [22]) relies on the application of absorbing chain techniques [27, pp. 128-130] to compute hitting times. On the contrary, by specifying S(G) in terms of elements of the Moore-Penrose inverse of the asymmetric Laplacian in (7), there is a reduction in computer execution time: absorbing chain techniques are based on the iterative inversion of as many matrices as there are nodes in the network. Instead, our approach

⁷Note that $S(G)^{-1}$ is not a measure of harmonic centrality (see [23]), as our harmonic mean is based on $C_{rw}(j)$ scores, which are the reciprocal of node distances $\bar{H}(j)$, i.e. the expected hitting times associated to each target node j.

allows to obtain all relevant magnitudes by computing only *one* (generalised) inverse matrix for the whole network.

As an illustration, we depict the evolution of S(G) for the WTN throughout 1997-2015, comparing it to effective resistance indices computed on undirected and unweighted WTN setups. Data comes from the OECD Bilateral Trade by Industry and End Use (BTDIxE) database.⁸ We considered a subset of 93 countries continuously present within the timespan analysed.⁹ The transition probability matrices obtained from the WTN are irreducible, thus, our graphs are strongly connected. Moreover, in order to allow for consistency in our temporal analysis, we rescaled weights by setting Vol(G) = 1 when dealing with weighted networks (see [26]).¹⁰

Table 4 and Figure 3 report the results. Columns [4] – [9] of Table 4 show the Kirchhoff-type descriptor and its reciprocal for three different data setups: (i) weighted, directed; (ii) weighted, undirected and (iii) unweighted, undirected WTN. The second graph on the right-hand side panel of Figure 3 plots columns [5], [7] and [9], comparing random walk closeness centrality across setups. Note from the Table that the coefficient of variation (CV) of (the reciprocal of) our DW-Kirchhoff index (column [5]) shows the highest relative variability, as is evinced from the graph. On the contrary, the CV associated to the index for the unweighted/undirected case (column [9]) is only 0.023, i.e. the range of change in the index has been only 1/10 of the change in 1/S(G). The weighted/undirected index, though evincing similar direction of change to that of the DW-Kirchhoff index, has a comparatively

⁸Data can be accessed at:

http://www.oecd.org/trade/bilateraltradeingoodsbyindustryandend-usecategory.htm.

The empirical exercise has been implemented using the R statistical programming environment. Data and source code for reproducibility purposes are available from the authors upon request.

⁹These 93 countries represent at least 93.7% of the volume of world trade in all years considered. The remaining countries have been gathered in a residual 'Rest of the World' region.

¹⁰Thus, our focus is on capturing changes in the *structure* of the trading network, separating these from the evolution of aggregate trade volumes. Moreover, by normalising Vol(G) = 1 and keeping the number of nodes constant, $S(G)^{-1}$ precisely corresponds to a global measure of random walk (closeness) centrality.

¹¹Note that column [9] is plotted in a secondary y-axis, to visually inspect its evolution in the same plot. However, its range of change is comparatively limited.

reduced amplitude of fluctuations (its associated CV being only 40% that of $S(G)^{-1}$).

Table 4: World GDP growth, Trade Volumes and Kirchhoffian Descriptors (1997-2015)

[1]	[2]	[3]	[4]	[5]	[6]	[7]	[8]	[9]	
	(Graph weights:	Wei	Weighted		Weighted		Unweighted	
	G	raph direction:	Dir	ected	Undi	Undirected		Undirected	
Year	g_{GDP}	Trade Vol.	S(G)	1/S(G)	S(G)	1/S(G)	R(G)	1/R(G)	
	(in p.p.)	$(in 10^9 USD)$	$(in 10^6)$	$(in 10^{-8})$	$(in 10^6)$	$(in 10^{-8})$		$(in 10^{-2})$	
1997	3.73	5363.9	26.72	3.74	28.31	3.53	102.33	0.977	
1998	2.54	5347.3	22.93	4.36	26.48	3.78	100.78	0.992	
1999	3.22	5614.7	27.51	3.64	29.37	3.40	101.11	0.989	
2000	4.34	6398.1	31.51	3.17	32.05	3.12	99.04	1.010	
2001	1.97	6178.7	29.51	3.39	32.23	3.10	98.92	1.011	
2002	2.21	6438.3	30.17	3.31	32.69	3.06	98.56	1.015	
2003	2.95	7526.0	27.30	3.66	33.76	2.96	98.14	1.019	
2004	4.33	9176.3	25.85	3.87	33.30	3.00	98.02	1.020	
2005	3.83	10406.0	25.09	3.99	31.87	3.14	97.64	1.024	
2006	4.30	12019.2	24.38	4.10	31.78	3.15	96.72	1.034	
2007	4.21	13815.0	22.10	4.52	30.63	3.26	96.23	1.039	
2008	1.79	15922.7	22.28	4.49	33.04	3.03	95.79	1.044	
2009	-1.72	12195.7	17.68	5.66	27.96	3.58	95.89	1.043	
2010	4.30	15006.3	19.96	5.01	30.32	3.30	95.77	1.044	
2011	3.16	17875.9	19.60	5.10	27.81	3.60	95.42	1.048	
2012	2.45	18033.5	19.96	5.01	27.64	3.62	95.33	1.049	
2013	2.59	18402.1	24.92	4.01	32.37	3.09	94.84	1.054	
2014	2.83	18347.3	18.02	5.55	28.37	3.52	95.08	1.052	
2015	2.77	16080.9	14.94	6.69	24.94	4.01	94.85	1.054	
Descriptive Statistics									
Min	-1.72	5347.28	14.94	3.17	24.94	2.96	94.84	0.98	
Max	4.34	18402.12	31.51	6.69	33.76	4.01	102.33	1.05	
Mean	2.94	11586.73	23.71	4.38	30.26	3.33	97.39	1.03	
STDev	1.41	4995.40	4.58	0.92	2.59	0.30	2.27	0.02	
CV	0.480	0.431	0.193	0.211	0.086	0.089	0.023	0.023	

Source: Authors' computation based on OECD BTDIxE Database and UNSD National Accounts Database.

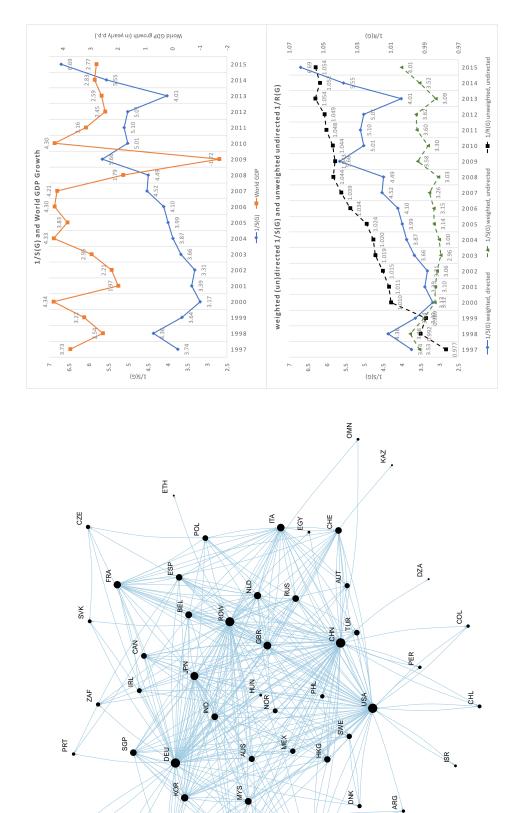


Figure 3: Application of Kirchhoffan descriptors to the analysis of the World Trade Network (1997-2015). Left-hand side panel: graph of a subset of the network of international trade in goods for 2015 (the plot shows only the subset of links representing at least 0.05% of world trade each. Taken together they cover 75% of total trade). Right-hand side panel: graphs depicting the evolution of 1/S(G) with respect to the growth rate of World GDP (above) and a comparison between Kirchhoff indices in three different setups: weighted/directed, weighted/undirected and unweighted/undirected variants of the world trade network (below).

Data sources: OECD Bilateral Trade by Industry and End Use Database (BTDIXE) and United Nations National Accounts Main Aggregates Database.

The importance of these differences in capturing the volatility in the structure of world trade becomes clear when comparing average random walk (closeness) centrality to the dynamics of world GDP (column [2] in Table 4). The first graph on the right-hand side panel of Figure 3 depicts columns [2] and [5] of the table. It evinces how the build-up of increasingly higher (average) closeness centrality up to the Great Recession of 2009 was followed by a sharp decline, which only returned (close) to its pre-crisis level in 2014. Thus, while an asset in good times, having a relatively low value of S(G) may render the world economy more fragile on a trade cycle downswing because countries are, on average, faster to be reached. Such a depiction could *not* have been portrayed with either the weighted/undirected or unweighted/undirected indices.¹²

Understandably, by taking into account all available information on inter-country flows (weight and direction), the DW-Kirchhoff index captures demand weaknesses in some spots of the world economy that become blurred when trade flows are rendered symmetric (by averaging import and export bilateral links) or binarised (by ignoring their relative importance). Thus, as this empirical illustration shows, the DW-Kirchhoff index may have a meaningful interpretation as a synthetic indicator of closeness centrality across nodes, within the context of random walks on graphs.

Differently from the DW-Kirchhoff index S(G) — which is intended to provide a synthetic global measure — the DW-multiplicative Kirchhoff index $S^*(G)$ may be used to uncover node-specific features. To see this, departing from (13), noting that it is valid for any i (thus, also for their average), and recalling that Vol(G) = 1 in our WTN application, we write:

$$S^*(G) = \sum_{j=1}^n \pi_j H(i,j) = \sum_{j=1}^n \pi_j \left(\frac{\sum_{i=1}^n H(i,j)}{n} \right) = \sum_{j=1}^n \pi_j \overline{H}(j) = \sum_{j=1}^n \frac{\overline{H}(j)}{(1/\pi_j)}$$
(22)

Inspecting (22), note that the DW-multiplicative Kirchhoff index can be recognised as an expression for Kemeny's constant [13]. More interestingly, it is the sum of individual node contributions. Each such contribution represents a ratio between the average hitting

¹²As can be confirmed by inspecting their almost uninterrupted upward trend or mild fluctuations.

time $\overline{H}(j)$ and the mean recurrence time $1/\pi_j$ [27], i.e. how immediately reachable a target node j is from all other source nodes, with respect to the time a random walker employs to depart from and return to node j.

Thus, within the WTN, a node contribution which is smaller than one $(\overline{H}(j) < 1/\pi_j)$ indicates that the country is immediately reachable from other nodes, on average, relatively faster than from itself, implying a lower aggregate indicator $S^*(G)$. On the contrary, a value greater than one $(\overline{H}(j) > 1/\pi_j)$ indicates that a country has a relatively lower mean recurrence time with respect to how immediately may be reached from other source nodes, implying a higher aggregate descriptor. Intuitively, the faster a country is reachable from other partners rather than from itself conveys the idea of dense interconnectedness amongst economies, and is reflected in a lower aggregate value of $S^*(G)$. Therefore, the addenda of the DW-multiplicative Kirchhoff index allow, for example, to build country rankings according to their individual contribution and compare these through time.¹³

The preference of S(G) over $S^*(G)$ as a global descriptor stems from the fact that each country's contribution to $S^*(G)$ is of the same order of magnitude, so a single node may have a crucial influence on the resulting aggregate score. Moreover, the range of variability of $S^*(G)$ through time is bound to be limited when compared to S(G), as evinced by figure 4 and columns [5]-[6] from table 5: when measured as a ratio with respect to the average across years, S(G) depicts clear-cut yearly changes, whereas deviations of $S^*(G)$ from unity are negligible.

Finally, note that the decomposition of the DW-additive Kirchhoff index $S^+(G)$ in (19) has S(G) and $S^*(G)$ as key components. In the WTN application, for Vol(G) = 1, S(G)/n is of the order 1×10^5 , whereas $nS^*(G)$ and $n\boldsymbol{\pi}^T\mathbf{M}\boldsymbol{\pi}$ are each of the order 1×10^3 . Thus, the evolution of S(G) dominates over the other two additive components, and the correlation between $S^+(G)$ and S(G) is almost 1, allowing us to focus on S(G) as the global indicator of interest in this WTN application.

 $^{^{13}}$ Though an interesting avenue for further research, such an exploration would take us beyond the scope of the present paper, mostly focused on global Kirchhoffian descriptors.

 $^{^{14}\}mathrm{As}$ may be corroborated by inspecting columns [5] and [7] of Table 5.

Table 5: Comparison of Kirchhoffian descriptors, World Trade Network (1997-2015)

[1]	[2]	[3]	[4]	[5]	[6]	[7]		
	Or	iginal ur	Rat	Ratio with respect				
				to average				
Year	S(G)	$S^*(G)$	$S^+(G)$	S(G)	$S^*(G)$	$S^+(G)$		
	$(in 10^6)$		$(in 10^4)$					
1997	26.72	93.95	29.61	1.13	1.0025	1.12		
1998	22.93	93.84	25.54	0.97	1.0014	0.97		
1999	27.51	93.77	30.46	1.16	1.0006	1.15		
2000	31.51	93.74	34.77	1.33	1.0003	1.32		
2001	29.51	93.70	32.62	1.24	0.9999	1.24		
2002	30.17	93.70	33.32	1.27	0.9999	1.26		
2003	27.30	93.74	30.24	1.15	1.0002	1.15		
2004	25.85	93.74	28.68	1.09	1.0002	1.09		
2005	25.09	93.75	27.85	1.06	1.0004	1.06		
2006	24.38	93.74	27.09	1.03	1.0002	1.03		
2007	22.10	93.80	24.64	0.93	1.0009	0.93		
2008	22.28	93.77	24.84	0.94	1.0006	0.94		
2009	17.68	93.67	19.89	0.75	0.9995	0.75		
2010	19.96	93.66	22.34	0.84	0.9994	0.85		
2011	19.60	93.67	21.95	0.83	0.9995	0.83		
2012	19.96	93.60	22.34	0.84	0.9988	0.85		
2013	24.92	93.62	27.67	1.05	0.9990	1.05		
2014	18.02	93.58	20.26	0.76	0.9986	0.77		
2015	14.94	93.54	16.94	0.63	0.9981	0.64		
		Desc	eriptive Sta	tistics				
Mean	23.71	93.71	26.37	1.00	1.0000	1.00		

Source: Authors' computation based on OECD BTDIxE Database.

5. Concluding remarks

We have provided a generalisation of three Kirchhoff-type global indices — namely the Kirchhoff index, the multiplicative and the additive Kirchhoff indices — for strongly connected, weighted digraphs. Following a probabilistic approach, we specified the generalised indices in terms of hitting and commute times, elements of the Moore-Penrose inverses and

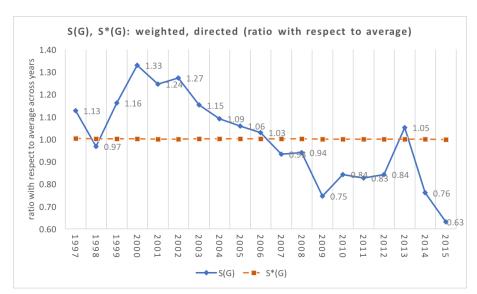


Figure 4: Ratio with respect to average across years: S(G) and $S^*(G)$, World Trade Network (1997-2015)

trace-cum-eigenvalues of alternative graph Laplacian matrices. We showed that, for the directed case, the Kirchhoff index can no longer correspond to a robustness measure, suggesting an alternative interpretation. In fact, by means of an empirical application to the World Trade Network, we showed how S(G), the generalised Kirchhoff-type descriptor introduced, provided a useful tool to study closeness centrality within the framework of Random Walks on graphs. Complementarily, within our empirical application, we compared the synthetic global indicator S(G) to a generalised multiplicative Kirchhoff index $S^*(G)$, which instead may be used to uncover node-specific features. We also noted, within this context, how the evolution of the generalised additive Kirchhoff index $S^+(G)$ is crucially determined by the Kirchhoff-type descriptor S(G).

At least two avenues of further research could be pursued.

On the one hand, a deeper exploration into Kirchhoff-type descriptors for directed, weighted networks that evince a monotonic behaviour when adding an edge (or increasing the weight of an existing link) is in place. Numerical examples considered depict an interesting pattern: in the event of adding a new link, the average hitting time of the nodes to which no new link was added increases. Formal exploration of this (and other) patterns for the case of weighted, directed graphs is a challenging issue we expect to tackle in future

work.

On the other hand, due to the continuously growing volume of empirical networks which are weighted and directed, applications of these Kirchhoff-type descriptors may include economic networks of different sorts (e.g. inter-industry production relations, firms' ownership structures, banks' financial balance sheets). If the analytical framework holds, applications in these directions (and others) may suitably follow.

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