Linear Algebra and its Applications 513 (2017) 201–209

Contents lists available at ScienceDirect

Linear Algebra and its Applications

www.elsevier.com/locate/laa

On the Ihara zeta function and resistance distance-based indices

Marius Somodi

Department of Mathematics, University of Northern Iowa, Cedar Falls, IA 50614, USA

A R T I C L E I N F O

Article history:
Received 18 August 2016
Accepted 26 September 2016
Available online 29 September 2016
Submitted by R. Brualdi

MSC:
05C50
05C12
05C07

Keywords:
Ihara zeta function
Resistance distance
Kirchhoff index

A B S T R A C T

We show that the Ihara zeta function of a graph determines a resistance distance-based invariant which is a linear combination of the Kirchhoff index, additive degree-Kirchhoff index, and multiplicative degree-Kirchhoff index.

1. Introduction

Let G be a graph of order n and size m. G may have parallel edges and/or loops. The Ihara zeta function of G is a function of complex argument defined, for $|u|$ sufficiently small, by

$$Z_G(u) = \prod_{[C]} (1 - u^{\nu([C])})^{-1},$$

E-mail address: marius.somodi@uni.edu.

http://dx.doi.org/10.1016/j.laa.2016.09.042
0024-3795/

where $[C]$ runs over all the prime cycles of G and $\nu([C])$ denotes the length of $[C]$. We refer the reader to [25] for an in-depth treatment of zeta functions of graphs.

Bass [1] showed that the Ihara zeta function satisfies the following determinant formula:

$$Z_G(u)^{-1} = (1-u^2)^{m-n} \det(\mathbf{I}_n - u\mathbf{A} + u^2(\mathbf{D} - \mathbf{I}_n))$$

where $\mathbf{A}$ and $\mathbf{D}$ are the adjacency and degree matrices of G, respectively.

The zeta function of a connected graph G that is md2 (i.e. it has no pendant vertices) encodes several invariants of the graph, including its order, size, number of loops, girth, and complexity (the number of spanning trees). In addition, Z_G determines whether G is regular, bipartite, or a circuit graph and, for particular classes of graphs, determines the graph's adjacency spectrum [8,9,14,23].

Motivated by the theory of electrical networks, Klein and Randic [16] introduced a distance function on a simple connected graph G, subsequently called the *resistance distance*: the resistance distance between a pair of vertices v_i and v_j of G is the effective resistance r_{ij} between v_i and v_j, when G is regarded as an electrical network with unit resistors placed on each edge.

Using the resistance distance metric, a graph invariant called the *Kirchhoff index* was defined [5,16] as

$$Kf = \sum_{1 \le i < j \le n} r_{ij}.$$

More recently, two other resistance distance-based graph invariants were put forward: the *additive degree-Kirchhoff index* [12], defined as

$$Kf^+ = \sum_{1 \le i < j \le n} (d_i + d_j) r_{ij}$$

and the *multiplicative degree-Kirchhoff index* [6], defined as

$$Kf^* = \sum_{1 \le i < j \le n} d_i d_j r_{ij}$$

where d_i and d_j are the degrees of the vertices v_i and v_j.

A small sample of recent articles about the three invariants is [3,4,7,10,15,17,20–22, 26,27].

If $\mathrm{Spec}_L(G) = \{\mu_1 = 0, \mu_2, ..., \mu_n\}$ and $\mathrm{Spec}_N(G) = \{\nu_1 = 0, \nu_2, ..., \nu_n\}$ are the Laplacian and normalized Laplacian spectra of G, respectively, then [6,13]

$$Kf = n \sum_{i=2}^{n} \frac{1}{\mu_i} \tag{1}$$

and

$$Kf^* = 2m\sum_{i=2}^{n}\frac{1}{\nu_i}. \tag{2}$$

The additive degree-Kirchhoff index can be determined using a probabilistic approach (see [19,20] for details): define a random walk on a simple connected graph G of order n, size m, and degree sequence $d_1, d_2, ..., d_n$, as the n-state Markov chain with transition matrix $\mathbf{P} = (p_{ij})$, where $p_{ij} = \dfrac{1}{d_i}$, if vertices v_i and v_j are neighbors, and 0 otherwise. The stationary distribution $\pi = (\pi_i)_{1\le i\le n}$ of the chain is given by $\pi_i = \dfrac{d_i}{2m}$. Let $\mathbf{W}$ be the $n \times n$ matrix whose rows are all equal to π. If T_j denotes the hitting time of vertex v_j and E_iT_j is the expected value of T_j when the walk starts at vertex v_i then, as shown in [20],

$$Kf^+ = \sum_{i=1}^{n}\sum_{j\neq i}\pi_j E_iT_j + \sum_{j=1}^{n}\sum_{i\neq j}\pi_i E_iT_j. \tag{3}$$

It is known that $E_iT_j = \dfrac{z_{jj} - z_{ij}}{\pi_j}$, where z_{ij} are the entries of the fundamental matrix $\mathbf{Z} = (\mathbf{I}_n - \mathbf{P} + \mathbf{W})^{-1}$.

A natural question is whether the Ihara zeta function determines any of these Kirchhoffian indices. While, for arbitrary graphs, the answer is no, in this note we show that the Ihara zeta function of an md2 graph encodes a resistance distance-based invariant defined as

$$\sum_{1\le i<j\le n}(d_i - 2)(d_j - 2)r_{ij}.$$

2. Main results

For the rest of the note, G is a connected md2 graph that may have parallel edges and/or loops. If we order the vertices $v_1, ..., v_n$ of G, then the adjacency matrix of G is an $n \times n$ matrix $\mathbf{A} = (a_{ij})$, where a_{ij} = the number of edges between v_i and v_j, if $i \neq j$, and a_{ii} = twice the number of loops at vertex v_i. The degree matrix of G is the diagonal matrix $\mathbf{D} = \mathrm{diag}(d_1, ..., d_n)$, where d_i = the number of first neighbors of vertex v_i plus twice the number of loops at vertex v_i. The Laplacian matrix of G is the matrix $\mathbf{L} = \mathbf{D} - \mathbf{A}$.

The resistance distance in a simple connected graph can be expressed in terms of the minors of its Laplacian matrix [2]: if $i \neq j$ then

$$r_{ij} = \frac{\det \mathbf{L}^{(ij)}}{\tau} \tag{4}$$

where $\mathbf{L}^{(ij)}$ is the matrix obtained from $\mathbf{L}$ by deleting its ith and jth rows and columns and τ denotes the complexity of G; if $i = j$ then $r_{ii} = 0$. We use (4) to define the resistance distance in connected graphs with parallel edges and/or loops. This allows us to extend the definitions of the three Kirchhoffian indices to such graphs.

In addition, we define (for md2 graphs)

$$Kf^z = \sum_{1 \le i < j \le n} (d_i - 2)(d_j - 2) r_{ij}.$$

Note that, if G is r-regular, then $Kf^z = (r-2)^2 Kf$. In general, for arbitrary connected graphs,

$$Kf^z = Kf^* - 2Kf^+ + 4Kf.$$

If G has one or more loops at each vertex, then $Kf^z(G) = Kf^*(G')$, where G' is the graph obtained from G by deleting one loop from each vertex.

Northshield [18] showed that, for a graph G of order n, size m, adjacency matrix $\mathbf{A}$, and degree matrix $\mathbf{D}$, if $f(u) = \det(\mathbf{I}_n - u\mathbf{A} + u^2(\mathbf{D} - \mathbf{I}_n))$ then

$$f'(1) = 2(m-n)\tau.$$

In light of Northshield's result, it is natural to ask if the second derivative of f encodes any important information about the graph.

Theorem 2.1. *Let G be an md2 graph of order n, size m, complexity τ, with adjacency matrix $\mathbf{A}$ and degree matrix $\mathbf{D}$. If $f(u) = \det(\mathbf{I}_n - u\mathbf{A} + u^2(\mathbf{D} - \mathbf{I}_n))$ then*

$$f''(1) = 2(Kf^z + 2mn - 2n^2 + n)\tau.$$

Proof. We proceed like in [18]. Let

$$f(u) = \det(\mathbf{I}_n - u\mathbf{A} + u^2(\mathbf{D} - \mathbf{I}_n)) = \det((1-u^2)\mathbf{I}_n + u\mathbf{L} + (u^2 - u)\mathbf{D})$$

where $\mathbf{L} = (l_{ij})$ is the Laplacian matrix of G and

$$\mathbf{M}(u) = (1-u^2)\mathbf{I}_n + u\mathbf{L} + (u^2 - u)\mathbf{D}.$$

For $1 \le p \le n$, let $\mathbf{M}_p(u)$ be the matrix obtained by differentiating the pth row of $\mathbf{M}(u)$. Then

$$\det(\mathbf{M}(u))' = \sum_{p=1}^{n} \det(\mathbf{M}_p(u)).$$

Note that the entry (i,j) of $\mathbf{M}_p(u)$ is

$$m_{p,ij} = (1 - ud_i + u^2(d_i - 1))\delta_{ij} + ul_{ij} + \\ + [((3d_i - 2)u - (d_i - 1)u^2 - d_i - 1)\delta_{ij} + (1-u)l_{ij}]\delta_{ip}$$

where δ_{ij} denotes the Kronecker symbol.

For $1 \le p \ne q \le n$, let $\mathbf{M}_{pq}(u)$ be the matrix obtained by differentiating the pth and qth rows of $\mathbf{M}(u)$. In addition, let $\mathbf{M}_{pp}(u)$ be the matrix obtained by differentiating twice the pth row of $\mathbf{M}(u)$. Then

$$f''(1) = \sum_{p=1}^{n} \det(\mathbf{M}_{pp}(1)) + 2 \sum_{1 \le p < q \le n} \det(\mathbf{M}_{pq}(1)). \tag{5}$$

Since the non-diagonal entries on the pth row of $\mathbf{M}(u)$ are linear in u, then the pth row of $\mathbf{M}_{pp}(1)$ has all the entries equal to 0 except for the diagonal entry, which is $2(d_p - 1)$. It follows that

$$\det(\mathbf{M}_{pp}(1)) = 2(d_p - 1)\det \mathbf{L}^{(p)},$$

where $\mathbf{L}^{(p)}$ is the matrix obtained from $\mathbf{L}$ by deleting its pth row and column. By the matrix-tree theorem, $\det \mathbf{L}^{(p)} = \tau$. Therefore

$$\sum_{p=1}^{n} \det(\mathbf{M}_{pp}(1)) = (4m - 2n)\tau. \tag{6}$$

Now let $1 \le p < q \le n$. Then

$$\mathbf{M}_{pq}(1) = \mathbf{L} + (d_p - 2)\mathbf{S}_p + (d_q - 2)\mathbf{S}_q,$$

where $\mathbf{S}_p = (s_{ij})$, with $s_{ij} = \delta_{ij}\delta_{ip}$. Note that

$$\det(\mathbf{L} + (d_p - 2)\mathbf{S}_p + (d_q - 2)\mathbf{S}_q) = \\ = \det(\mathbf{L} + (d_q - 2)\mathbf{S}_q) + (d_p - 2)\det(\mathbf{L}^{(p)} + (d_q - 2)\mathbf{S}_q^{(p)}) \tag{7}$$

where $\mathbf{S}_q^{(p)}$ is the matrix obtained from $\mathbf{S}_q$ by deleting its pth row and column.

Using the matrix-tree theorem,

$$\det(\mathbf{L} + (d_q - 2)\mathbf{S}_q) = \det \mathbf{L} + (d_q - 2)\det \mathbf{L}^{(q)} = (d_q - 2)\tau$$

and

$$\det(\mathbf{L}^{(p)} + (d_q - 2)\mathbf{S}_q^{(p)}) = \det \mathbf{L}^{(p)} + (d_q - 2)\det \mathbf{L}^{(pq)} = \tau + (d_q - 2)\det \mathbf{L}^{(pq)}.$$

Therefore, according to (7)

$$\det(\mathbf{L} + (d_p - 2)\mathbf{S}_p + (d_q - 2)\mathbf{S}_q) =$$
$$= (d_p + d_q - 4)\tau + (d_p - 2)(d_q - 2)\det \mathbf{L}^{(pq)}$$

which, by (4), can be expressed as

$$(d_p + d_q - 4)\tau + (d_p - 2)(d_q - 2)r_{pq}\tau.$$

It follows that

$$\sum_{1 \le p < q \le n} \det(\mathbf{M}_{pq}(1)) = \sum_{1 \le p < q \le n} (d_p + d_q - 4)\tau + \sum_{1 \le p < q \le n} (d_p - 2)(d_q - 2) r_{pq}\tau =$$
$$= [(2m - 2n)(n - 1) + Kf^z]\tau. \tag{8}$$

The desired equality follows from (5), (6), and (8). □

The corollary from [18] shows that

$$\lim_{u \to 1^-} Z_G(u)^{-1}(1 - u)^{n-m-1} = -2^{m-n+1}(m - n)\tau.$$

Corollary 2.2.

$$\lim_{u \to 1^-} \frac{Z_G(u)^{-1}(1 - u)^{n-m-1} + 2^{m-n+1}(m - n)\tau}{1 - u} =$$
$$= 2^{m-n}(Kf^z + m^2 - n^2 + n)\tau.$$

Proof. Note that

$$Z_G(u)^{-1}(1 - u)^{n-m-2} = (1 - u^2)^{m-n} f(u)(1 - u)^{n-m-2} = \frac{(1 + u)^{m-n} f(u)}{(1 - u)^2}$$

so

$$\lim_{u \to 1^-} [Z_G(u)^{-1}(1 - u)^{n-m-2} + \frac{2^{m-n+1}(m - n)\tau}{1 - u}] =$$
$$= \lim_{u \to 1^-} [\frac{(1 + u)^{m-n} f(u)}{(1 - u)^2} + \frac{2^{m-n+1}(m - n)\tau}{1 - u}] =$$
$$= \lim_{u \to 1^-} \frac{(1 + u)^{m-n} f(u) + 2^{m-n+1}(m - n)\tau(1 - u)}{(1 - u)^2}.$$

Since $f(1) = \det \mathbf{L} = 0$, the previous limit equals

$$\lim_{u \to 1^-} \frac{(m - n)(1 + u)^{m-n-1} f(u) + (1 + u)^{m-n} f'(u) - 2^{m-n+1}(m - n)\tau}{-2(1 - u)}.$$

Using the Theorem from [18], $f'(1) = 2(m-n)\tau$ so the previous limit equals

$$\frac{1}{2}[(m-n)2^{m-n}f'(1) + 2^{m-n}f''(1)] = 2^{m-n-1}[2(m-n)^2\tau + f''(1)] = \\ = 2^{m-n}[Kf^z + m^2 - n^2 + n]\tau. \quad \square$$

Since the Ihara zeta function of an md2 connected graph encodes the graph's order, size, and complexity, it follows that the Ihara zeta function also determines the graph's Kf^z invariant.

The question arises whether the Ihara zeta function of an arbitrary connected md2 graph determines Kf, Kf^+, or Kf^*. The answer to this question is no. Durfee and Martin found two simple connected md2 graphs ("the crab" and "the squid") that have the same Ihara zeta function but different degree sequences (see Example 2.2 from [11]). We calculated the Ihara zeta functions of the two graphs (all computations summarized in this note were done using Sage) and found

$$Z(u)^{-1} = (48u^{15} + 72u^{13} - 8u^{12} + 64u^{11} - 12u^{10} + 41u^9 - 8u^8 + 22u^7 - 5u^6 + 10u^5 - \\ - 2u^4 + 5u^3 - 2u^2 - 1)(u^2+u+1)^2(u^2-u+1)(u^2+1)(u^2-1)^4(u-1).$$

We also determined the Laplacian and normalized Laplacian characteristic polynomials of the crab and the squid graphs and, by (1) and (2), calculated the Kirchhoff and multiplicative degree-Kirchhoff indices of each graph using Viete's relations. In addition, we determined the fundamental matrix $\mathbf{Z}$ and calculated the additive degree-Kirchhoff index of each graph using (3). The results are summarized below:

$$\text{Crab graph}: Kf = \frac{607}{7}, \quad Kf^+ = \frac{9166}{21}, \quad Kf^* = \frac{22,843}{42}$$
$$\text{Squid graph}: Kf = \frac{593}{7}, \quad Kf^+ = \frac{8956}{21}, \quad Kf^* = \frac{22,339}{42}$$

Combining the three Kirchhoffian indices (or using the Ihara zeta function), we find that both the crab and the squid have $Kf^z = \frac{249}{14}$.

Corollary 2.3. *Let G and H be connected md2 graphs that have one or more loops at each vertex and G' and H' be the graphs obtained from G and H by deleting one loop from each vertex. If $Z_G = Z_H$ then $Kf^*(G') = Kf^*(H')$.*

Czarneski found a pair of non-isomorphic graphs, with loops at each vertex, that have the same Ihara zeta function [9, Figure 2.3]:

$$Z(u)^{-1} = (240u^5 - 232u^4 + 139u^3 - 51u^2 + 13u - 1)(u-1)(1-u^2)^9.$$

These graphs have $Kf^z = 43$, so the graphs obtained from them by deleting one loop from each vertex have the same multiplicative degree-Kirchhoff index ($Kf^* = 43$).

Let $S(G)$ be the subdivision graph of a simple graph G, i.e. the graph obtained from G by adding one vertex to each edge. Yang and Klein [26] expressed the three Kirchhoffian indices of $S(G)$ in terms of the three Kirchhoffian indices of G. Using their results (Theorems 2.3, 2.4, and 2.5), we get

$$Kf^z(S(G)) = 2Kf^z(G) \tag{9}$$

and

$$Kf(S(G)) = \frac{1}{2}Kf^z(G) + 2Kf^+(G) + \frac{1}{2}(m^2 - n^2 + n). \tag{10}$$

The equality from display (10) leads to:

Remark 2.4. Let G and H be simple connected md2 graphs that have the same order, size, and $Kf^z(G) = Kf^z(H)$ (all these conditions are satisfied if G and H have the same Ihara zeta function). Then $Kf^+(G) = Kf^+(H)$ if and only if $Kf(S(G)) = Kf(S(H))$.

We recall that Setyadi and Storm [24] enumerated (up to an isomorphism) all the simple connected md2 graphs on up to 11 vertices and calculated their Ihara zeta functions. They found a unique pair of non-isomorphic md2 graphs of order 8 that have the same Ihara zeta function (see Figure 2 from [24]):

$$\begin{aligned} Z(u)^{-1} = {} & (144u^{11} + 24u^{10} + 172u^9 + 98u^7 - 9u^6 + 45u^5 - 3u^4 + 12u^3 - 3u^2 + u - 1) \times \\ & \times (3u^2 + u + 1)(2u^2 + u + 1)(1 - u^2)^6(u - 1). \end{aligned}$$

Using Sage, we found that their graphs have the same additive degree-Kirchhoff index. Therefore, by the previous remark, their subdivision graphs (which have order 22) have the same Kirchhoff index and, from (9), the same Kf^z invariant. The Kirchhoffian indices of Setyadi and Storm's graphs are:

$$\begin{aligned} &Kf(G) = 19.70, \quad Kf^*(G) = 220.4, \quad Kf^+(G) = 132.6, \quad Kf^z(G) = 34 \\ &Kf(H) = 19.75, \quad Kf^*(H) = 220.2, \quad Kf^+(H) = 132.6, \quad Kf^z(H) = 34 \end{aligned}$$

(all the values are exact). We also note that $S(G)$ and $S(H)$ have different additive degree-Kirchhoff indices and different multiplicative degree-Kirchhoff indices. This follows from Theorems 2.4 and 2.5 [26], as G and H have the same additive degree-Kirchhoff index but different multiplicative degree-Kirchhoff indices.

Acknowledgements

The author would like to thank the referee and George Cazacu for their suggestions and comments.

References

[1] H. Bass, The Ihara–Selberg zeta function of a tree lattice, Internat. J. Math. 3 (1992) 717–797.
[2] R.B. Bapat, I. Gutman, W. Xiao, A simple method for computing resistance distance, Z. Naturforsch. 58a (2003) 494–498.
[3] E. Bendito, A. Carmona, A.M. Encinas, J.M. Gesto, A formula for the Kirchhoff index, Int. J. Quantum Chem. 108 (2008) 1200–1206.
[4] M. Bianchi, A. Cornaro, J.L. Palacios, A. Torriero, Bounds for the Kirchhoff index via majorization techniques, J. Math. Chem. 51 (2013) 569–587.
[5] D. Bonchev, A.T. Balaban, X. Liu, D.J. Klein, Molecular cyclicity and centricity of polycyclic graphs: I. Cyclicity based on resistance distances or reciprocal distances, Int. J. Quantum Chem. 50 (1) (1994) 1–20.
[6] H. Chen, F. Zhang, Resistance distance and the normalized Laplacian spectrum, Discrete Appl. Math. 155 (2007) 654–661.
[7] Z. Cinkir, Contraction formulas for the Wiener and Kirchhoff indices, MATCH Commun. Math. Comput. Chem. 75 (2016) 169–198.
[8] Y. Cooper, Properties determined by the Ihara zeta function of a graph, Electron. J. Combin. 16 (2009) R84.
[9] D. Czarneski, Zeta function of graphs, PhD Dissertation, LSU, 2005.
[10] Q. Deng, H. Chen, On the Kirchhoff index of the complement of a bipartite graph, Linear Algebra Appl. 439 (2013) 167–173.
[11] C. Durfee, K. Martin, Distinguishing graphs with zeta functions and generalized spectra, Linear Algebra Appl. 481 (2015) 54–82.
[12] I. Gutman, L. Feng, G. Yu, Degree resistance distance of unicyclic graphs, Trans. Combin. 1 (2) (2012) 27–40.
[13] I. Gutman, B. Mohar, The quasi-Wiener and the Kirchhoff indices coincide, J. Chem. Inf. Comput. Sci. 36 (5) (1996) 982–985.
[14] M. Horton, Ihara zeta functions of digraphs, Linear Algebra Appl. 425 (2007) 130–142.
[15] J. Huang, S. Li, On the normalized Laplacian spectrum, degree-Kirchhoff index and spanning trees of graphs, Bull. Aust. Math. Soc. 91 (2015) 353–367.
[16] D.J. Klein, M. Randic, Resistance distance, J. Math. Chem. 12 (1993) 81–95.
[17] I. Milovanovic, I. Gutman, E. Milovanovic, On Kirchhoff and degree Kirchhoff indices, Filomat 29 (8) (2015) 1869–1877.
[18] S. Northshield, A note on the zeta function of a graph, J. Combin. Theory Ser. B 74 (1998) 408–410.
[19] J.L. Palacios, Resistance distance in graphs and random walks, Int. J. Quantum Chem. 81 (2001) 29–33.
[20] J.L. Palacios, Upper and lower bounds for the additive degree-Kirchhoff index, MATCH Commun. Math. Comput. Chem. 70 (2013) 651–655.
[21] J.L. Palacios, Some interplay of the three Kirchhoffian indices, MATCH Commun. Math. Comput. Chem. 75 (2016) 199–206.
[22] J.L. Palacios, J.M. Renom, Another look at the degree-Kirchhoff index, Int. J. Quantum Chem. 111 (2011) 3453–3455.
[23] G. Scott, C. Storm, The coefficients of the Ihara zeta function, Involve 1 (2) (2008) 217–233.
[24] A. Setyadi, C.K. Storm, Enumeration of graphs with the same Ihara zeta function, Linear Algebra Appl. 438 (2013) 564–572.
[25] A. Terras, Zeta Functions of Graphs: A Stroll Through the Garden, Cambridge U. Press, 2011.
[26] Y. Yang, D.J. Klein, Resistance distance-based graph invariants of subdivisions and triangulations of graphs, Discrete Appl. Math. 181 (2015) 260–274.
[27] H. Zhang, Y. Yang, C. Li, Kirchhoff index of composite graphs, Discrete Appl. Math. 157 (2009) 2918–2927.