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Computing the Additive Degree–Kirchhoff Index with the Laplacian Matrix

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ABSTRACT

For any simple connected undirected graph, it is well known that the Kirchhoff and multiplicative degree–Kirchhoff indices can be computed using the Laplacian matrix. We show that the same is true for the additive degree–Kirchhoff index and give a compact Matlab program that computes all three Kirchhoffian indices with the Laplacian matrix as the only input.

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1. INTRODUCTION

Let $G = (V, E)$ be a finite simple connected graph with vertex set $V = \{1,2,\cdots,n\}$ and degrees d_i for $1 \leq i \leq n$. The general formula

$$R^f(G) = \sum_{\{i<j\}} f(i,j) R_{\{ij\}}, \qquad (1)$$

where $R_{\{ij\}}$ is the effective resistance between vertices i and j and $f(i,j)$ is some real function of the vertices, identifies a family of descriptors widely studied in Mathematical Chemistry. Among these, the ones that have undergone a more intense scrutiny are the Kirchhoff index R(G), the multiplicative degree–Kirchhoff index $R^*(G)$ and the additive degree–Kirchhoff index $R^+(G)$ defined by (1) when taking $f(i,j) = 1$, $f(i,j) = d_i d_j$ and $f(i,j) = d_i + d_j$, respectively, and introduced in [10], [3] and [6] respectively. The references [9, 12, 17−20] are a recent sample of works where some interesting relationships between these three indices are highlighted.

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A possible approach to compute these indices is to find first the individual values $R_{\{ij\}}$ and then compute the sums in (1). It is well known (see [2]), for instance, that

$$R_{\{ij\}} = L^{\#}{}_{\{ii\}} + L^{\#}{}_{\{jj\}} - L^{\#}{}_{\{ij\}} - L^{\#}{}_{\{ji\}}, \tag{2}$$

where $\boldsymbol{L}^{\#}$ is the Moore–Penrose inverse of the Laplacian matrix $\mathbf{L} = \mathbf{D} - \mathbf{A}$, $\mathbf{D}$ is the diagonal matrix with the degrees of the vertices in the diagonal, and $\mathbf{A}$ is the adjacency matrix of G. It is also known (see [2]) that the resistances can be expressed in terms of the Laplacian matrix:

$$R_{\{ij\}} = \frac{\det \mathbf{L}(i,j)}{\det \mathbf{L}(i)}, \tag{3}$$

where $\mathbf{L}$(i,j) and $\mathbf{L}$(i) are obtained from $\mathbf{L}$ by deleting its $i-th$ row and $j-th$ column, and by deleting its $i-th$ row and column, respectively.

This approach, though amenable to being programmed, does not seem to be computationally efficient, because it entails computing n^2+n determinants just to get the values of the effective resistances. If in addition we want to compute the additive degree–Kirchhoff index, besides storing the matrix $\mathbf{L}$ we need to store the matrix of resistances $\mathbf{R} = R_{\{ij\}}$ in order to compute $\sum_{\{i,j\}} d_i d_j R_{\{ij\}}$ with an additional set of additions and multiplications.

A major breakthrough in the computation of these indices is the fact that two of them have a simple expression in terms of certain eigenvalues, namely (see [7, 21]), and also [8] and [15] for alternative proofs)

$$R(G) = n\sum_{i=1}^{n-1}\frac{1}{\lambda_i} \tag{4}$$

for $\lambda_1 \geq \cdots \geq \lambda_{n-1} > \lambda_n = 0$ the eigenvalues of the Laplacian matrix. Likewise (see [3])

$$R^*(G) = 2|E|\sum_{i=1}^{n-1}\frac{1}{\beta_i}, \tag{5}$$

for $2 \geq \beta_1 \geq \cdots \geq \beta_{n-1} > \beta_n = 0$ the eigenvalues of the normalized Laplacian matrix $\boldsymbol{\mathcal{L}} = \mathbf{D}^{\frac{-1}{2}}\mathbf{L}\mathbf{D}^{\frac{-1}{2}}$, and also (see [16])

$$R^*(G) = 2|E|\sum_{i=2}^{n}\frac{1}{1-\alpha_i} \tag{6}$$

for $1 = \alpha_1 > \alpha_2 \geq \cdots \geq \alpha_n \geq -1$ the eigenvalues of the transition probability matrix $\mathbf{P} = \mathbf{D}^{-1}\mathbf{A}$ of the random walk on G.

There is a probabilistic connection between effective resistances and random walks on graphs that allow us to express $R(G)$ in terms of the fundamental matrix $\mathbf{Z}$ of the random walk on G (see [14]), $R^*(G)$ in terms of the eigenvalues of $\mathbf{P}$, as in(6), and $R^+(G)$ as a more involved expression

$$R^{+}(G) = \frac{1}{d_G} R^{*}(G) + \sum_{j} \sum_{i} \pi_i E_i T_j, \tag{7}$$

where $\pi = (\pi_i)_{1 \le i \le n}$ is the stationary distribution of the random walk on G, which can be given explicitly as $\pi_i = \frac{d_i}{2|E|}$, and where $E_i T_j$ denotes the expected hitting time of the vertex j by the walk on G started at the vertex i (see [1] for all matters regarding random walks on graphs). In principle, one could use the expression (7) to compute $R^{+}(G)$, but in addition to working with **L** for the calculation of $R^{*}(G)$, we need to store **Z,** then compute the hitting times and store them in an additional matrix from which the sum $\sum_j \sum_i \pi_i E_i T_j$ can be computed with additional operations.

In [20] and [9] they came up, almost simultaneously, with the same idea of expressing

$$R^{+}(G) = d_G R(G) + n \operatorname{trace}(\mathbf{D}\mathbf{L}^{\#}). \tag{8}$$

Calculating $R^{+}(G)$ with (8) is perfectly feasible. A possible concern is the complexity in the calculation of the Moore Penrose inverse. More on this below.
Also recently (see [18]), we found that

$$R^{+}(G) = \frac{1}{d_G} R^{*}(G) + 2|E| \sum_{i=1}^{n} \frac{1}{\upsilon_i} - n, \tag{9}$$

where the $\upsilon_i s$ are the eigenvalues of the modified Laplacian matrix $\mathbf{L} + \mathbf{DW}$, and **W** is the matrix all of whose rows are copies of the stationary distribution π^T defined above.

The interesting point now is to realize that the new modified Laplacian matrix can be written exclusively in terms of the Laplacian matrix: indeed, the matrix **D** is the diagonal matrix whose elements are those in the diagonal of **L** (see below the simple Matlab command to get **D** from **L**) and

$$\boldsymbol{W} = \frac{1}{2|E|} \mathbf{OD}$$

where **O** is the $n \times n$ matrix of all whose entries are ones. In what follows we will use for the computation of the Kirchhoffian indices only the formulas (4),(5) and (9) where in the last equation, the $\upsilon_i s$ are the eigenvalues of the invertible matrix $\mathbf{L} + \frac{1}{2|E|}\mathbf{DOD}$.

2. THE COMPUTATIONS

Clearly (4), (5) and (9) depend exclusively on **L**. Perhaps this is more evident if we write 2|E| trace **L**=trace **D**.

Also, the sums of inverses of eigenvalues in (4),(5) and (9) can be written as

$$\sum_{i=1}^{n-1} \frac{1}{\lambda_i} = -\frac{a_2}{a_1} \tag{10}$$

$$\sum_{i=1}^{n-1} \frac{1}{\beta_i} = -\frac{b_2}{b_1} \tag{11}$$

and

$$\sum_{i=1}^{n} \frac{1}{\nu_i} = -\frac{c_1}{c_0} \tag{12}$$

where a_i, i = 1, 2 (resp. b_i, i=1, 2 and c_i, i = 0, 1) are the coefficients of x^i in the characteristic polynomial of **L** (resp. $\boldsymbol{\mathcal{L}}$ and $\mathbf{L} + \frac{1}{2|E|}\mathbf{DOD}$).

To see for instance that (10) holds, we notice that:

$$\sum_{i=1}^{n-1} \frac{1}{\lambda_i} = \frac{\sum \lambda_{i_1}\lambda_{i_2} \cdots \lambda_{i_{n-2}}}{\lambda_1\lambda_2 \cdots \lambda_{n-1}}$$

where the sum in the numerator runs over all (n–2)–long products of distinct nonzero eigenvalues. We then apply Vieta's formulas (see [13]) for the sums of products of the roots of a polynomial in terms of its coefficients. Formulas (11) and (12) follow similarly.

We will now write the Matlab commands to obtain the three indices when the only input is the Laplacian matrix of the graph. Matlab is a registered trademark of the Mathworks [11].

Once **L** has been entered, no other matrix needs to be manipulated, and these are the commands used (with a brief comment of their purpose in the parentheses):

>>[n,n]=size(L) (recovers the number of vertices of the graph)

>>a=flip(charpoly(L)) (finds the vector of coefficients $a(i)$ of x^{i-1},$1 \le i \le n+1$ for the characteristic polynomial of L)

>>R1 $= -n * \frac{a(3)}{a(2)}$ (finds the Kirchhoff index)

>>D = diag(diag(L)) (finds the diagonal matrix D)

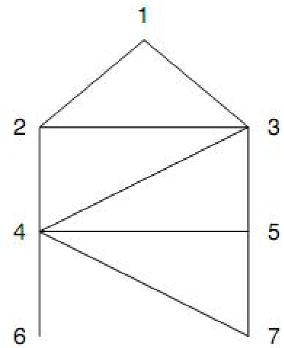
>>b = flip(charpoly($D \wedge (\frac{-1}{2}) * L * D \wedge (\frac{-1}{2})$)) (finds the vector of coefficients b(i) of x^{i-1},$1 \le i \le n+1$ for the characteristic polynomial of $\boldsymbol{\mathcal{L}}$

>>R2 $= -\mathrm{trace}(L) * \frac{b(3)}{b(2)}$ (finds the multiplicative degree–Kirchhoff index)

>> c = flip(charpoly(L+1/trace(D)*D*ones(n)*D)) (finds the vector of coefficients $c(i)$ of x^{i-1}, $1 \le i \le n+1$, for the characteristic polynomial of $\mathbf{L} + \frac{1}{2|E|}\mathbf{DOD}$

>>R3 $= n * R2/trace(D) - trace(D) * c(2)/c(1) - n$ (finds the additive degree–Kirchhoff index)

For illustration purposes we will use the graph in the following figure.



Once the matrix **L** has been entered, Matlab returns the vectors

a:

0 385 −1106 1181 −600 156 −20 1

b:

0 1.5278 −9.4944 23.3194 −29.2417 19.8917 −7.0000 1.0000

c:

1.0e+03*

−1.1000 3.6284 −4.6636 3.0416 −1.0985 0.2219 −0.0234 0.0010

and the indices R1 = 20.1091, R2 = 124.2909, R3 = 102.4727.

Final remarks. A question may arise as to the advantages of using formula (9) instead of (8) when computing $R^{+}(G)$. We can point to the fact that the computation of the characteristic polynomial of the matrix $\mathbf{L} + \frac{1}{2|E|}\mathbf{DOD}$ is done in Matlab using the well studied Hessenberg's algorithm (see [4]) with the command "charpoly", and the computation of the Moore–Penrose inverse with the command "pinv" of Matlab, and other algorithms, is cause for concern as to the time and space requirements. Indeed, both "charpoly" and "pinv" are of order $O(n^3)$, but the constant of the n^3 term seems to be much larger in the case of the "pinv" command (see [5]).

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