A Simple Method for Computing Resistance Distance

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The resistance distance r_{ij} between two vertices v_i and v_j of a (connected, molecular) graph G is equal to the effective resistance between the respective two points of an electrical network, constructed so as to correspond to G, such that the resistance of any edge is unity. We show how r_{ij} can be computed from the Laplacian matrix L of the graph G: Let $L(i)$ and $L(i,j)$ be obtained from L by deleting its i-th row and column, and by deleting its i-th and j-th rows and columns, respectively. Then $r_{ij} = \det L(i,j)/\det L(i)$.

Key words: Resistance Distance; Laplacian Matrix; Kirchhoff Index; Molecular Graph.

1. Introduction

When the structure of a molecule is represented by a metric topological space [1 – 5], then the distance between two vertices v_i and v_j, denoted by d_{ij}, is defined as the length (= number of edges) of a shortest path that connects v_i and v_j in the corresponding molecular graph G. The vertex-distance concept found numerous chemical applications; for details see the recent reviews [6 – 8] and elsewhere [9 – 11]. In order to examine other possible metrics in (molecular) graphs, Klein and Randić [12] conceived the *resistance distance* between the vertices of a graph G, denoted by r_{ij}, defined to be equal to the effective electrical resistance between the nodes i and j of a network N corresponding to G, with unit resistors taken over any edge of N. For acyclic graphs $r_{ij} = d_{ij}$, and therefore the resistance distances are primarily of interest in the case of cycle-containing (molecular) graphs.

Resistance-distances and molecular structure-descriptors based on them were much studied in the chemical literature [12 – 23] and recently attracted the attention also of mathematicians [24, 25]. In analogy to the classical Wiener index [7 – 11], one introduced [12] the sum of resistance distances of all pairs of vertices of a molecular graph,

$$Kf = \sum_{i<j} r_{ij}, \qquad (1)$$

a structure-descriptor that eventually was named [13] the "*Kirchhoff index*".

Resistance distances are computed by methods of the theory of resistive electrical networks (based on Ohm's and Kirchhoff's laws); for details see [24]. The standard method to compute r_{ij} is via the Moore-Penrose generalized inverse $L^\dagger$ of the Laplacian matrix L of the underlying graph G:

$$r_{ij} = (L^\dagger)_{ii} + (L^\dagger)_{jj} - (L^\dagger)_{ij} - (L^\dagger)_{ji}. \qquad (2)$$

Equation (2) is stated already in [12] and [14], but was, for sure, known much earlier.

In this work we communicate a novel, remarkably simple expression for r_{ij}, stated in Theorem 1. In order to be able to formulate our main result, we first specify our notation and terminology and remind the readers to some basic facts from Laplacian graph spectral theory.

2. On Laplacian Spectral Theory

Let G be a graph and let its vertices be labeled by $v_1, v_2, \ldots, v_n$. The Laplacian matrix of G, denoted by $L = L(G)$, is a square matrix of order n whose (i,j)-entry is defined by

$L_{ij} = -1$, if $i \neq j$ and the vertices v_i and v_j are adjacent,
$L_{ij} = 0$, if $i \neq j$ and the vertices v_i and v_j are not adjacent,
$L_{ij} = d_i$, if $i = j$,

where d_i is the degree (= number of first neighbors) of the vertex v_i.

Because $\sum_{i=1}^{n} L_{ij} = \sum_{j=1}^{n} L_{ij} = 0$ for any graph G, $\det L(G) = 0$, i. e., $L(G)$ is singular.

The submatrix obtained from the Laplacian matrix L by deleting its i-th row and the i-th column will be denoted by $L(i)$. The submatrix obtained from the Laplacian matrix L by deleting its i-th and j-th rows and the i-th and j-th columns will be denoted by $L(i,j)$, assuming that $i \neq j$.

According to the famous matrix-tree theorem (see for instance [26 – 29]) for any graph G and for any $i = 1, 2, \ldots, n$,

$$\det L(i) = t(G), \tag{3}$$

where $t(G)$ is the number of spanning trees of G.

The eigenvalues of the Laplacian matrix are referred to as the Laplacian eigenvalues and form the Laplacian spectrum of the respective graph. The Laplacian spectral theory is a well elaborated part of algebraic graph theory and its details can be found in numerous reviews, for instance in [27, 30, 31]. Concerning chemical applications of Laplacian spectra see [32, 33].

We label the Laplacian eigenvalues of the graph G by μ_i, $i = 1, 2, \ldots, n$, so that

$$\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n.$$

Then, μ_n is always equal to zero, whereas μ_{n-1} differs from zero if and only if the underlying graph G is connected. (We are interested in molecular graphs, which necessarily are connected. Therefore in what follows it will be understood that $\mu_{n-1} \neq 0$.)

Of the many known relations between the structure of a graph and its Laplacian spectrum [26 – 28, 30 – 33] we mention here only two:

$$\prod_{i=1}^{n-1} \mu_i = n\,t(G) \tag{4}$$

and

$$Kf = n \sum_{i=1}^{n-1} \frac{1}{\mu_i}. \tag{5}$$

3. A Determinantal Formula for r_{ij}

Theorem 1. *Let G be a connected graph on n vertices, $n \geq 3$, and $1 \leq i \neq j \leq n$. Let $L(i)$ and $L(i,j)$ be the above defined submatrices of the Laplacian matrix of the graph G. Then*

$$r_{ij} = \frac{\det L(i,j)}{\det L(i)}. \tag{6}$$

In view of (3), formula (6) can be written also as

$$r_{ij} = \frac{\det L(i,j)}{t(G)}.$$

This remarkably simple expression for the resistance distance was discovered by one of the present authors [25]. Here we demonstrate its validity in a manner different from that in [25].

In order to prove Theorem 1 we need some preparations.

To each vertex v_i of the graph G associate a variable x_i and consider the auxiliary function

$$f(x_1, x_2, \ldots, x_n) = \sum_{k,\ell} (x_k - x_\ell)^2$$

with the summation going over all pairs of adjacent vertices v_k, v_ℓ. Then for $i \neq j$,

$$r_{ij} = \sup \left\{ \frac{1}{f(x_1, x_2, \ldots, x_n)} \,\middle|\, x_i = 1, x_j = 0, 0 \leq x_k \leq 1, \right.$$
$$\left. k = 1, 2, \ldots, n \right\}. \tag{7}$$

Formula (7) is a result known in the theory of electrical networks (cf. Corollary 5 on p. 301 in Chapt. 9 of the book [24]). Its immediate consequences are the following equations which hold for $k \neq i, j$:

$$\frac{\partial f}{\partial x_k} = 2 \sum_{\ell \in \Gamma(k)} (x_k - x_\ell) = 0, \tag{8}$$

where $\Gamma(k)$ denotes the set of first neighbors of the vertex v_k.

Because the vertices of the graph G are labeled in an arbitrary manner, without loss of generality we may restrict our considerations to the special case $i = n-1$ and $j = n$. Then, however, the mathematical formalism of our analysis will become significantly simpler.

For the sake of simplicity, denote the submatrix $L(n-1, n)$ by L_{n-2} and write the Laplacian matrix of G as

$$L(G) = \begin{pmatrix} L_{n-2} & B \\ C & D \end{pmatrix}.$$

Then (8) can be written as

$$L_{n-2}\boldsymbol{x}^t = \boldsymbol{b}^t, \tag{9}$$

where $\boldsymbol{x} = (x_1, x_2, \ldots, x_{n-2})$ and $\boldsymbol{b} = (b_1, b_2, \ldots, b_{n-2})$. Because $x_{n-1} = 1$ and $x_n = 0$, if the vertices v_{n-1} and v_k are adjacent then $b_k = 1$, whereas otherwise $b_k = 0$, $k = 1, 2, \ldots, n-2$.

Let $A = ||a_{ij}||$ be the adjacency matrix of the graph G. Then, in view of $x_{n-1} = 1$, $x_n = 0$, in addition to (9) we have

$$\boldsymbol{x}B(x_{n-1}, x_n)^t = (x_{n-1}, x_n)C\boldsymbol{x}^t = -\sum_{i=1}^{n-2} a_{n-1,i}x_i \tag{10}$$

and

$$(x_{n-1}, x_n)D(x_{n-1}, x_n)^t = d_{n-1}. \tag{11}$$

By combining (9)–(11) we obtain

$$\begin{aligned} &f(x_1, x_2, \ldots, x_n) \\ &\quad = (\boldsymbol{x}, x_{n-1}, x_n)L(G)(\boldsymbol{x}, x_{n-1}, x_n)^t \\ &\quad = \boldsymbol{x}L_{n-2}\boldsymbol{x}^t + (x_{n-1}, x_n)C\boldsymbol{x}^t \\ &\qquad + \boldsymbol{x}B(x_{n-1}, x_n)^t + (x_{n-1}, x_n)D(x_{n-1}, x_n)^t \\ &\quad = \boldsymbol{x}\boldsymbol{b}^t - 2\sum_{i=1}^{n-2} a_{n-1,i}x_i + d_{n-1}. \end{aligned}$$

Because

$$\boldsymbol{x}\boldsymbol{b}^t = \sum_{i=1}^{n-2} a_{n-1,i}x_i = \sum_{k\in\Gamma(n-1)} x_k,$$

we finally arrive at the relation

$$f(x_1, x_2, \ldots, x_n) = d_{n-1} - \sum_{k\in\Gamma(n-1)} x_k, \tag{12}$$

which holds under the extreme value condition $x_{n-1} = 1$, $x_n = 0$.

The matrix $L(G)$ is positive semidefinite. If the graph G is connected, then the matrix L_{n-2} is positive definite. Thus its inverse $(L_{n-2})^{-1}$ exists. Let the (i,j)-entry of $(L_{n-2})^{-1}$ be denoted by t_{ij}. Then, $\boldsymbol{x}^t = (L_{n-2})^{-1}\boldsymbol{b}^t$, implying

$$x_k = \sum_{\ell\in\Gamma(n-1)} t_{k\ell}. \tag{13}$$

Proof of Theorem 1. As already explained, it is sufficient to demonstrate the validity of Theorem 1 for $i = n-1$ and $j = n$.

By (12) and (13) we have under the extreme value condition

$$f(x_1, x_2, \ldots, x_n) = d_{n-1} - \sum_{k\in\Gamma(n-1)} \sum_{\ell\in\Gamma(n-1)} t_{k\ell}. \tag{14}$$

Let $L_{n-2}(k,\ell)$ be the submatrix obtained by removing from L_{n-1} the k-th row and the ℓ-th column. Then,

$$t_{k\ell} = (-1)^{k+\ell}\,\frac{\det L_{n-2}(k,\ell)}{\det L_{n-2}}.$$

Thus by (14)

$$\begin{aligned} &f(x_1, x_2, \ldots, x_n) \qquad (15) \\ &\quad = d_{n-1} - \sum_{k\in\Gamma(n-1)} \sum_{\ell\in\Gamma(n-1)} (-1)^{k+\ell}\frac{\det L_{n-2}(k,\ell)}{\det L_{n-2}}. \end{aligned}$$

By expanding $\det L(n)$ with respect to its last column we get

$$\begin{aligned} \det L(n) &= d_{n-1}\det L_{n-2} \\ &\quad - \sum_{k\in\Gamma(n-1)} (-1)^{k+n-1}\det L(n)(k, n-1), \end{aligned}$$

where the submatrix $L(n)(k, n-1)$ is obtained by removing the k-th row and the $(n-1)$-th column of $L(n)$. Further, expanding $\det L(n)(k, n-1)$ with respect its last row,

$$\det L(n)(k, n-1) = \sum_{\ell\in\Gamma(n-1)} (-1)^{\ell+n-1}\det L_{n-2}(k,\ell).$$

This yields

$$\begin{aligned} &d_{n-1}\det L_{n-2} - \sum_{k\in\Gamma(n-1)} \sum_{\ell\in\Gamma(n-1)} (-1)^{k+\ell}\det L_{n-2}(k,\ell) \\ &\quad = \det L(n), \end{aligned}$$

which substituted back into (15) becomes

$$f(x_1, x_2, \ldots, x_n) = \frac{\det L(n)}{\det L_{n-2}}. \tag{16}$$

Theorem 1 follows when (16) is substituted back into (7). □

4. Applications

The most obvious and probably the most useful application of formula (6) is in a simple procedure for computing resistance distances. If $\mu'_1, \mu'_2, \ldots, \mu'_{n-1}$ and $\mu''_1, \mu''_2, \ldots, \mu''_{n-2}$ are the eigenvalues of the submatrices $L(i)$ and $L(i,j)$, respectively, then

$$\det L(i) = \prod_{r=1}^{n-1} \mu'_r, \tag{17}$$

$$\det L(i,j) = \prod_{r=1}^{n-2} \mu''_r, \tag{18}$$

and r_{ij} is readily obtained. As far as algorithm complexity is concerned, the usage of (17) and (18) is not the most efficient way to compute resistance distances. However, the method is extremely simple for writing a computer program (provided, of course, that a software for matrix diagonalization is available).

Corollary 1.1. *For any connected n-vertex graph, $n \geq 2$, the Kirchhoff index (1), is expressed in terms of Laplacian eigenvalues as (5).*

Proof. Suppose that the Laplacian characteristic polynomial of G, defined as $\psi(G,\lambda) = \det(\lambda I_n - L(G))$, where I_n is the unit matrix of order n, is written as

$$\psi(G,\lambda) = \sum_{k=0}^{n} (-1)^k c_k \lambda^{n-k}.$$

Then all the coefficients c_k are non-negative integers and, inparticular [24, 26]

$$c_n = 0,$$

$$c_{n-1} = nt(G), \text{ c. f. (4)},$$

$$c_{n-2} = \left(\prod_{j=1}^{n-1} \mu_j\right)\left(\sum_{i=1}^{n-1} \frac{1}{\mu_i}\right) = nt(G) \sum_{i=1}^{n-1} \frac{1}{\mu_i}.$$

The Kirchhoff index is defined via (1). Then by Theorem 1,

$$Kf = \sum_{i<j} r_{ij} = \sum_{i<j} \frac{\det L(i,j)}{t(G)} = \frac{c_{n-2}}{t(G)} \quad = n \sum_{i=1}^{n-1} \frac{1}{\mu_i}. \square$$

Formula (5) was reported earlier (for details and further references see [7, 33]), but was deduced by a completely different way of reasoning.

Since r_{ij} is a distance function [25], we obtain by Theorem 1:

Corollary 1.2. *If i, j, k are distinct to each other, then* $\det L(i,k) \leq \det L(i,j) + \det L(j,k)$.

If i, j are distinct, then by the well-known Hadamard-Fisher inequality

$$\det L(i) \leq d_i \det L(i,j) \ .$$

Thus from Theorem 1 immediately follows

Corollary 1.3.

$$r_{ij} \geq \max\left\{\frac{1}{d_i}, \frac{1}{d_j}\right\}.$$

In the below Theorem 2 we deduce a better lower, and also an upper bound for the resistance distance.

From (9) we get

$$\boldsymbol{b}(L_{n-2})^{-1}\boldsymbol{b}^t = \boldsymbol{b}\boldsymbol{x}^t = \sum_{k=1}^{n-2} b_k x_k = \sum_{k \in \Gamma(n-1)} x_k.$$

Then by (12),

$$f(x_1, x_2, \ldots, x_n) = d_{n-1} - \boldsymbol{b}(L_{n-2})^{-1}\boldsymbol{b}^t. \tag{19}$$

Evidently, if the vertices v_n and v_{n-1} are adjacent then $d_{n-1} = \boldsymbol{b}\boldsymbol{b}^t + 1$, otherwise $d_{n-1} = \boldsymbol{b}\boldsymbol{b}^t$.

Let I_{n-2} be the unit matrix of order $n-2$. Then by (19) we obtain

$$f(x_1, x_2, \ldots, x_n) = \boldsymbol{b}[I_{n-2} - (L_{n-2})^{-1}]\boldsymbol{b}^t \tag{20}$$

if the vertices v_n and v_{n-1} are not adjacent. Otherwise

$$f(x_1, x_2, \ldots, x_n) = \boldsymbol{b}\left[\frac{d_{n-1}}{d_{n-1}-1} I_{n-2} - (L_{n-2})^{-1}\right]\boldsymbol{b}^t. \tag{21}$$

As before, the eigenvalues of the matrix $L(i,j)$ are denoted by

$$\mu''_1 \geq \mu''_2 \geq \cdots \geq \mu''_{n-2} > 0.$$

Then, of course, $1/\mu''_i$, $i = 1, 2, \ldots, n-2$, are the eigenvalues of $(L_{n-2})^{-1}$. Then from (20) and (21) and by taking into account (7) follows:

Theorem 2. *Let $i \neq j$. If the vertices v_i and v_j are not adjacent, then*

$$d_i\left(1 - \frac{1}{\mu''_{n-2}}\right) \leq \frac{1}{r_{ij}} \leq d_i\left(1 - \frac{1}{\mu''_1}\right)$$

and

$$\frac{\mu_1''}{d_i(\mu_1''-1)} \le r_{ij} \le \frac{\mu_{n-2}''}{d_i(\mu_{n-2}''-1)}$$

with the upper bound for r_{ij} applicable only if $d_i(\mu_{n-2}''-1)>0$, i. e., $\mu_{n-2}''>1$.

Otherwise

$$d_i\left(1-\frac{1}{\mu_{n-2}''}\right)+\frac{1}{\mu_{n-2}''} \le \frac{1}{r_{ij}} \le d_i\left(1-\frac{1}{\mu_1''}\right)+\frac{1}{\mu_1''}$$

and

$$\frac{\mu_1''}{d_i(\mu_1''-1)+1} \le r_{ij} \le \frac{\mu_{n-2}''}{d_i(\mu_{n-2}''-1)+1}$$

with the upper bound for r_{ij} applicable only if $d_i(\mu_{n-2}''-1)+1>0$, i. e., $\mu_{n-2}''>1-1/d_i$.

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