

The Quasi-Wiener and the Kirchhoff Indices Coincide

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In 1993 two novel distance-based topological indices were put forward. In the case of acyclic molecular graphs both are equal to the Wiener index, but both differ from it if the graphs contain cycles. One index is defined (Mohar, B.; Babić, D.; Trinajstić, N. *J. Chem. Inf. Comput. Sci.* **1993**, 33, 153–154) in terms of eigenvalues of the Laplacian matrix, whereas the other is conceived (Klein, D. J.; Randić, M. *J. Math. Chem.* **1993**, 12, 81–95) as the sum of resistances between all pairs of vertices, assuming that the molecule corresponds to an electrical network, in which the resistance between adjacent vertices is unity. Eventually, the former quantity was named quasi-Wiener index and the latter Kirchhoff index. We now demonstrate that the quasi-Wiener and Kirchhoff indices of all graphs coincide.

1. INTRODUCTION

The study of topological indices based on distances between the vertices of the molecular graph has been undergoing rapid expansion in the last few years. A large number of such indices was recently introduced and examined in due detail. Here we are concerned with two of them, namely with the quasi-Wiener index, W^* , and the Kirchhoff index, Kf . These have been conceived and investigated independently of each other, and, until now, no relation between them seems to have been noticed in the published chemical or mathematical literature.¹ We now show that W^* and Kf are, in fact, one and the same topological index, i.e., that the equality $W^* = Kf$ holds for all molecular graphs.

Let G be a molecular graph, possessing n vertices, v_1, v_2, \dots, v_n . By δ_i we denote the degree (= number of first neighbors) of the vertex v_i and by Δ the diagonal matrix of order n , whose diagonal elements are $\delta_1, \delta_2, \dots, \delta_n$. Then the Laplacian matrix of G is defined as

$$L = \Delta - A$$

where A is the adjacency matrix. The eigenvalues of L , denoted by $\lambda_1, \lambda_2, \dots, \lambda_n$, form the so-called Laplacian graph spectrum. Conventionally, these eigenvalues are labeled so that $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_{n-1} \geq \lambda_n$. The Laplacian spectrum has been extensively studied by mathematicians.^{2–5} Of the numerous properties known for this spectrum we mention the following:

- (a) The Laplacian eigenvalues are non-negative numbers.
- (b) The eigenvalue λ_n is always equal to zero.
- (c) The eigenvalue λ_{n-1} is greater than zero if and only if the graph G is connected.

Because of (b), the Laplacian matrix L is singular and, consequently, has no inverse. Molecular graphs are necessarily connected. Properties (a) and (c) imply that for such graphs the eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_{n-1}$ are positive numbers.

The following interesting result seems to have been discovered in the late 1980s by Brendan McKay^{3,6–8} (and later rediscovered by Merris^{6,9})

$$W = n \sum_{i=1}^{n-1} \frac{1}{\lambda_i} \quad (1)$$

where W stands for the Wiener index, i.e., for the sum of distances between all pairs of vertices of the graph G . Formula 1 holds only in the case of acyclic graphs.

The chemical community was made acquainted with formula 1 by means of the paper¹⁰ and review.¹¹ Some chemical applications of (1) were also reported.¹²

In the case of graphs containing cycles, the right-hand side of eq 1 is not equal to the Wiener index but is otherwise a well-defined quantity. The name “quasi-Wiener index” was proposed for it¹³ as well as the symbol W^* . The correlation between W and W^* was studied in the case of benzenoid molecules¹³ and found to be linear, but not particularly good.

Klein and Randić¹⁴ considered recently the so-called resistance distance between the vertices of a (molecular) graph G , which is equal to the resistance between two respective vertices of an electrical network, constructed so as to correspond to G , and having the property that the resistance of each bond joining adjacent vertices is unity. Then, in analogy to the Wiener index, one may examine the sum of resistance distances between all pairs of vertices. In the case of acyclic graphs this sum is, evidently, equal to the Wiener index, but in the case of graphs possessing cycles it differs from W . In the original work of Klein and Randić¹⁴ no name was given to the sum of resistance distances, but in a later article¹⁵ the very appropriate name “Kirchhoff index” was proposed,¹⁶ together with the symbol Kf . (Recall that the resistances as well as other fundamental properties of electrical networks are determined by the two classical laws of Kirchhoff.^{17,18})

Using the theory of electrical networks^{17,18} the authors of ref 14 showed that

$$Kf = n \operatorname{Tr} L^{-1} \quad (2)$$

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where Tr stands for the trace (= sum of diagonal entries) of \mathbf{L}^\dagger and where \mathbf{L}^\dagger is the so-called Moore–Penrose generalized inverse^{19,20} of the Laplacian matrix \mathbf{L} .²¹

The aim of this paper is to demonstrate that the right-hand sides of eqs 1 and 2 always coincide.

2. ON THE GENERALIZED INVERSE OF A SINGULAR MATRIX

As already pointed out, the Laplacian matrix \mathbf{L} is singular and therefore has no inverse. In other words, it is not possible to find a matrix \mathbf{L}^{-1} , such that $\mathbf{L} \mathbf{L}^{-1} = \mathbf{L}^{-1} \mathbf{L} = \mathbf{I}$, where \mathbf{I} is the unit matrix.

In the case of singular matrices, instead of inverses (which do not exist) one can sometimes use so-called generalized inverses. Several types of generalized inverses are known in the mathematical literature.^{19,20} In the theory of electrical networks the Moore–Penrose generalized inverse is encountered.²² Because this matter is not widely known among chemists, we outline it in some detail.

Let \mathbf{M} be a real, symmetric square matrix of order n . Then the eigenvalues of \mathbf{M} are real numbers. Let \mathbf{S}_0 be the vector space, spanned by those eigenvectors of \mathbf{M} whose eigenvalues are equal to zero. Let \mathbf{S}_+ be the vector space, spanned by the eigenvectors of \mathbf{M} whose eigenvalues are nonzero.

The Moore–Penrose generalized inverse of a matrix \mathbf{M} is denoted by \mathbf{M}^\dagger . In the case of symmetric square matrices, \mathbf{M}^\dagger is defined^{19,20} so that $\mathbf{M} \mathbf{M}^\dagger = \mathbf{M}^\dagger \mathbf{M}$ is an orthogonal projector on the vector space \mathbf{S}_+ . This means that it is required:

$$(\mathbf{M} \mathbf{M}^\dagger) \mathbf{u} = (\mathbf{M}^\dagger \mathbf{M}) \mathbf{u} = \mathbf{0} \quad \text{for all vectors } \mathbf{u} \in \mathbf{S}_0 \quad (3)$$

$$(\mathbf{M} \mathbf{M}^\dagger) \mathbf{v} = (\mathbf{M}^\dagger \mathbf{M}) \mathbf{v} = \mathbf{v} \quad \text{for all vectors } \mathbf{v} \in \mathbf{S}_+ \quad (4)$$

Conditions 3 and 4 uniquely determine \mathbf{M}^\dagger .

3. THE GENERALIZED INVERSE OF THE LAPLACIAN MATRIX

In what follows, the superscript T will indicate transposition. Thus, if $\mathbf{M} = ||M_{ij}||$, then $\mathbf{M}^T = ||M_{ji}||$. Further, if \mathbf{c} is a column-vector

$$\mathbf{c} = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{pmatrix}$$

then $\mathbf{c}^T = (c_1, c_2, \dots, c_n)$ is a row-vector.

A square matrix of order n , whose diagonal elements are b_1, b_2, \dots, b_n , and whose off-diagonal elements are zero will be denoted by $\text{diag}(b_1, b_2, \dots, b_n)$. In particular, $\Delta = \text{diag}(\delta_1, \delta_2, \dots, \delta_n)$.

Consider the Laplacian matrix \mathbf{L} of a connected graph. Let $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_{n-1}$ be the eigenvectors²³ of \mathbf{L} corresponding to the positive eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_{n-1}$. Let \mathbf{e} be the eigenvector²³ of \mathbf{L} corresponding to the (unique) zero eigenvalue λ_n of \mathbf{L} . In this case \mathbf{S}_+ is an $(n-1)$ -dimensional vector space, spanned by $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_{n-1}$. Because the eigenvectors of \mathbf{L} are mutually orthogonal, \mathbf{e} is orthogonal to any element of \mathbf{S}_+ . Thus, if $\mathbf{y} \in \mathbf{S}_+$, then the scalar product of \mathbf{e} and \mathbf{y} , denoted by $\mathbf{e}^T \mathbf{y}$, is equal to zero.

The Laplacian matrix is a real symmetric square matrix. Therefore, conditions 3 and 4 are applicable to its generalized inverse \mathbf{L}^\dagger , namely

$$(\mathbf{L} \mathbf{L}^\dagger) \mathbf{e} = (\mathbf{L}^\dagger \mathbf{L}) \mathbf{e} = \mathbf{0}$$

$$(\mathbf{L} \mathbf{L}^\dagger) \mathbf{y} = (\mathbf{L}^\dagger \mathbf{L}) \mathbf{y} = \mathbf{y} \quad \text{for all vectors } \mathbf{y}, \quad \mathbf{y} \in \mathbf{S}_+.$$

It is easy to verify that

$$\mathbf{L} \mathbf{L}^\dagger = \mathbf{I} - \mathbf{e} \mathbf{e}^T$$

where, as before, \mathbf{I} stands for the unit matrix of order n . Indeed,

$$(\mathbf{I} - \mathbf{e} \mathbf{e}^T) \mathbf{e} = \mathbf{I} \mathbf{e} - (\mathbf{e} \mathbf{e}^T) \mathbf{e} = \mathbf{e} - \mathbf{e} (\mathbf{e}^T \mathbf{e}) = \mathbf{e} - \mathbf{e} \cdot 1 = \mathbf{0}$$

$$(\mathbf{I} - \mathbf{e} \mathbf{e}^T) \mathbf{y} = \mathbf{I} \mathbf{y} - (\mathbf{e} \mathbf{e}^T) \mathbf{y} = \mathbf{y} - \mathbf{e} (\mathbf{e}^T \mathbf{y}) = \mathbf{y} - \mathbf{e} \cdot 0 = \mathbf{y}$$

Let $\mathbf{U} = (\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_{n-1}, \mathbf{e})$ be the unitary matrix, diagonalizing \mathbf{L} . Thus,

$$\mathbf{U} \mathbf{U}^T = \mathbf{U}^T \mathbf{U} = \mathbf{I}$$

and

$$\mathbf{U}^T \mathbf{L} \mathbf{U} = \underline{\Lambda} = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_{n-1}, \lambda_n)$$

Then

$$\mathbf{L} = \mathbf{U} \underline{\Lambda} \mathbf{U}^T \quad (5)$$

because of

$$\mathbf{U} \underline{\Lambda} \mathbf{U}^T = \mathbf{U} (\mathbf{U}^T \mathbf{L} \mathbf{U}) \mathbf{U}^T = (\mathbf{U} \mathbf{U}^T) \mathbf{L} (\mathbf{U} \mathbf{U}^T) = \mathbf{I} \mathbf{L} \mathbf{I} = \mathbf{L}$$

The main result on which the proof of the identity $W^* = Kf$ is based is the following formula

$$\mathbf{L}^\dagger = \mathbf{U} \underline{\Lambda}^\dagger \mathbf{U}^T \quad (6)$$

where

$$\underline{\Lambda}^\dagger = \text{diag}\left(\frac{1}{\lambda_1}, \frac{1}{\lambda_2}, \dots, \frac{1}{\lambda_{n-1}}, 0\right)$$

We now proceed to verify eq 6. Combining (5) and (6) we obtain

$$\begin{aligned} \mathbf{L} \mathbf{L}^\dagger &= (\mathbf{U} \underline{\Lambda} \mathbf{U}^T)(\mathbf{U} \underline{\Lambda}^\dagger \mathbf{U}^T) = \mathbf{U} \underline{\Lambda} (\mathbf{U}^T \mathbf{U}) \underline{\Lambda}^\dagger \mathbf{U}^T \\ &= \mathbf{U} \underline{\Lambda} \underline{\Lambda}^\dagger \mathbf{U}^T = \mathbf{U} \mathbf{J} \mathbf{U}^T \end{aligned}$$

where

$$\mathbf{J} = \text{diag}(1, 1, \dots, 1, 0)$$

It now remains to demonstrate that $\mathbf{U} \mathbf{J} \mathbf{U}^T$ is an orthogonal projector on the space \mathbf{S}_+ , i.e., that $\mathbf{U} \mathbf{J} \mathbf{U}^T = \mathbf{I} - \mathbf{e} \mathbf{e}^T$. For

this we have to show that

$$(\mathbf{U} \mathbf{J} \mathbf{U}^T) \mathbf{e} = \mathbf{0} \quad (7)$$

and

$$(\mathbf{U} \mathbf{J} \mathbf{U}^T) \mathbf{y} = \mathbf{y} \quad \text{for all } \mathbf{y}, \mathbf{y} \in \mathbf{S}_+. \quad (8)$$

Proof of Eq 7. Because \mathbf{e} is orthogonal to the other eigenvectors of \mathbf{L} , we have²³

$$\begin{aligned} \mathbf{e}^T \mathbf{U} &= \mathbf{e}^T (\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_{n-1}, \mathbf{e}) = \\ &= (\mathbf{e}^T \cdot \mathbf{x}_1, \mathbf{e}^T \cdot \mathbf{x}_2, \dots, \mathbf{e}^T \cdot \mathbf{x}_{n-1}, \mathbf{e}^T \cdot \mathbf{e}) \\ &= (0, 0, \dots, 0, 1) \end{aligned}$$

Therefore,

$$\mathbf{J} (\mathbf{e}^T \mathbf{U})^T = \begin{pmatrix} 1 & 0 \dots 0 & 0 \\ 0 & 1 \dots 0 & 0 \\ \dots & \dots & \dots \\ 0 & 0 \dots 1 & 0 \\ 0 & 0 \dots 0 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ \dots \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \dots \\ 0 \\ 0 \end{pmatrix} = \mathbf{0}$$

and

$$(\mathbf{U} \mathbf{J} \mathbf{U}^T) \mathbf{e} = \mathbf{U} [\mathbf{J} (\mathbf{e}^T \mathbf{U})^T] = \mathbf{U} \mathbf{0} = \mathbf{0}$$

which shows that condition 7 is obeyed.

Proof of Eq 8. Any vector belonging to the space \mathbf{S}_+ can be presented in the form

$$\mathbf{y} = \sum_{i=1}^{n-1} \alpha_i \mathbf{x}_i$$

where $\alpha_1, \alpha_2, \dots, \alpha_{n-1}$ are scalar multipliers. Because of the orthogonality of the eigenvectors of \mathbf{L}

$$\mathbf{y}^T \cdot \mathbf{x}_i = \alpha_i, i = 1, 2, \dots, n-1 \quad \text{and} \quad \mathbf{y}^T \cdot \mathbf{e} = 0$$

Therefore,

$$\mathbf{y}^T \mathbf{U} = \mathbf{y}^T (\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_{n-1}, \mathbf{e}) = (\alpha_1, \alpha_2, \dots, \alpha_{n-1}, 0)$$

Then

$$\begin{aligned} (\mathbf{U} \mathbf{J} \mathbf{U}^T) \mathbf{y} &= \mathbf{U} \mathbf{J} (\mathbf{y}^T \mathbf{U})^T = \mathbf{U} \begin{pmatrix} 1 & 0 \dots 0 & 0 \\ 0 & 1 \dots 0 & 0 \\ \dots & \dots & \dots \\ 0 & 0 \dots 1 & 0 \\ 0 & 0 \dots 0 & 0 \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \dots \\ \alpha_{n-1} \\ 0 \end{pmatrix} = \\ &= (\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_{n-1}, \mathbf{e}) \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \dots \\ \alpha_{n-1} \\ 0 \end{pmatrix} = \sum_{i=1}^{n-1} \mathbf{x}_i \alpha_i = \mathbf{y} \end{aligned}$$

and the validity of condition 8 is verified too.

By this we proved that \mathbf{L}^\dagger has the form 6.

$$4. W^* = \mathbf{Kf}$$

From (6) is evident that the eigenvalues of \mathbf{L}^\dagger are

$$\frac{1}{\lambda_1}, \frac{1}{\lambda_2}, \dots, \frac{1}{\lambda_{n-1}}, 0$$

Therefore,

$$\text{Tr } \mathbf{L}^\dagger = \sum_{i=1}^{n-1} \frac{1}{\lambda_i}$$

The fact that the Kirchhoff and the quasi-Wiener indices coincide follows now immediately from eqs 1 and 2.

By proving the identity $W^* = \mathbf{Kf}$ we gained a very easy method for computing the Kirchhoff index, namely via the eigenvalues of the Laplacian matrix, eq 1. The same identity reveals the hitherto obscure physical meaning of the quasi-Wiener index. However, in the time of rapid proliferation of topological indices, the main merit of the present work might be in reducing their number by one.

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REFERENCES AND NOTES

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- (16) In ref 15 the Kirchhoff index is defined as twice the sum of resistance distances between all pairs of vertices of a graph, being thus inconsistent with the usual definition of the Wiener index. In order

to maintain a full analogy with W , in this work we define the Kirchhoff index K_f as just the sum of resistance distances between all pairs of vertices. Then, in particular, $W = K_f$ holds for trees.

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- (21) Note that in ref 14 the generalized inverse of the Laplacian matrix is denoted by $Q/(\Delta - A)$. The present formula 2 is theorem F of ref 14. The symbol L^\dagger for the generalized inverse is taken from ref 19; it

should not be confused with the Hermitean conjugate, a notation often used in theoretical chemistry and theoretical physics.

- (22) The generalized inverse considered in this paper was first invented by R. H. Moore in 1935 but was eventually more or less forgotten. An equivalent concept was introduced by R. Penrose in 1955, who was apparently unaware of Moore's work. For additional details see pp 9–11 of ref 20.
- (23) The eigenvectors $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_{n-1}$, and \mathbf{e} are considered as column-vectors. They are assumed to be normalized, i.e., $\mathbf{x}_1^T \cdot \mathbf{x}_1 = \mathbf{x}_2^T \cdot \mathbf{x}_2 = \dots = \mathbf{x}_{n-1}^T \cdot \mathbf{x}_{n-1} = \mathbf{e}^T \cdot \mathbf{e} = 1$.

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