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Review

Mathematical Properties of Molecular Descriptors Based on Distances*

Bo Zhou[a,] and Nenad Trinajstić[b]**

[a]*Department of Mathematics, South China Normal University, Guangzhou 510631, P. R. China*
[b]*The Ruđer Bošković Institute, P. O. Box 180, HR-10002 Zagreb, Croatia*

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Abstract. A survey of a number of molecular descriptors based on distance matrices and distance eigenvalues is given. The following distance matrices are considered: the standard distance matrix, the reverse distance matrix, the complementary distance matrix, the resistance-distance matrix, the detour matrix, the reciprocal distance matrix, the reciprocal reverse Wiener matrix and the reciprocal complementary distance matrix. Mathematical properties are discussed for the following molecular descriptors with a special emphasis on their upper and lower bounds: the reverse Wiener index, the Harary index, the reciprocal reverse Wiener index, the reciprocal complementary Wiener index, the Kirchhoff index, the detour index, the Balaban index, the reciprocal Balaban index, the reverse Balaban index and the largest eigenvalues of distance matrices. This set of molecular descriptors found considerable use in QSPR and QSAR.

Keywords: Distance matrices, Wiener-like indices, distance eigenvalues, Balaban-like indices, upper and lower bounds, QSPR, QSAR

INTRODUCTION

Graph-theoretical matrices[1] and derived molecular descriptors[2,3] have played over the years important roles in QSPR and QSAR.[2–7] Among the variety of the graph-theoretical matrices proposed in the literature, the most important appear to be the (vertex-)adjacency matrix $\boldsymbol{A}$ and the (vertex-)distance matrix $\boldsymbol{D}$. The word vertex in front of both matrices indicates that these matrices are related to adjacencies and graph-theretical distances, respectively, between the vertices in the graph. However, in this report we shall not discuss the other pair of related matrices, that is, the edge-adjacency matrix and the edge-distance matrix; their definitions and application are detailed elsewhere.[1] Therefore, in this report we drop the word vertex from the names of both matrices and call them simply as the adjacency matrix and the distance matrix. These both matrices and their variants can serve as the generators for many different kinds of molecular descriptors that found extensive use in the structure-property-activity modeling.

In this report, we collect results on the mathematical aspects of some molecular descriptors, derived from the distance matrices presented above, especially regarding their upper and lower bounds. The bounds of a descriptor are important information on a molecule (graph) since they establish the approximate range of the applicability of the descriptor in QSPR and QSAR in terms of the molecular (graph-theoretical) structural parameters.

SURVEY OF MATRICES CONSIDERED

We consider simple graphs, i.e., graphs without loops and multiple edges.[8–10] Let G be a connected (molecular) graph with the vertex-set $V(G)=\{v_1,v_2,\ldots,v_n\}$ and edge-set $E(G)$.

The adjacency matrix $\boldsymbol{A}$ of G is an $n\times n$ matrix $(\boldsymbol{A}_{ij})$ such that $\boldsymbol{A}_{ij}=1$ if the vertices v_i and v_j are adjacent and 0 otherwise.[1,9,11] The distance matrix $\boldsymbol{D}$ of G is an $n\times n$ matrix $(\boldsymbol{D}_{ij})$ such that $\boldsymbol{D}_{ij}$ is just the distance (i.e., the number of edges of a shortest path) between the vertices v_i and v_j in G.[1,12,13] The diameter d of the graph G is the maximum possible distance between any two vertices in G.[8] The reverse Wiener matrix (or the reverse distance matrix) $\boldsymbol{RW}$ of G is an $n\times n$ matrix $(\boldsymbol{RW}_{ij})$ such that $\boldsymbol{RW}_{ij}=d-\boldsymbol{D}_{ij}$ if $i\neq j$, and 0 otherwise.[1,14] The complementary distance matrix $\boldsymbol{CD}$ of G is an $n\times n$ matrix $(\boldsymbol{CD}_{ij})$ such that $\boldsymbol{CD}_{ij}=1+d-\boldsymbol{D}_{ij}$ if $i\neq j$, and 0 otherwise.[1,15]

The resistance-distance matrix $\boldsymbol{R}$ of G is an $n\times n$ matrix $(\boldsymbol{R}_{ij})$ such that $\boldsymbol{R}_{ij}$ is equal to the resistance-distance between vertices v_i and v_j in G, which

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** Author to whom correspondence should be addressed. (E-mail: zhoubo@scnu.edu.cn)

is defined as the effective resistance between the respective two nodes of the electrical network obtained so that its nodes correspond to the vertices of G and each edge of G is replaced by a resistor of unit resistance, which is computed by the methods of the theory of resistive electrical networks based on Ohm's and Kirchhoff's laws.[1,16]

The detour matrix (or the maximum path matrix) $\boldsymbol{DM}$ of the graph G is an $n \times n$ matrix $(\boldsymbol{DM}_{ij})$ such that $\boldsymbol{DM}_{ij}$ is equal to the length of the longest distance between vertices v_i and v_j if $i \neq j$, and 0 otherwise.[1,9,17,18]

The reciprocal matrix ${}^{\mathrm{r}}\boldsymbol{M}$ of a symmetric $n \times n$ molecular matrix $\boldsymbol{M}$ is an $n \times n$ matrix $({}^{r}\boldsymbol{M}_{ij})$ such that ${}^{\mathrm{r}}\boldsymbol{M}_{ij} = \dfrac{1}{\boldsymbol{M}_{ij}}$ if $i \neq j$ and $\boldsymbol{M}_{ij} \neq 0$, and 0 otherwise. Then $\boldsymbol{RD} = {}^{\mathrm{r}}\boldsymbol{D}$ is the reciprocal distance matrix of G, also called the Harary matrix,[1,19,20] $\boldsymbol{RRW} = {}^{\mathrm{r}}\boldsymbol{RW}$ is the reciprocal reverse Wiener matrix[21] and $\boldsymbol{RCD} = {}^{\mathrm{r}}\boldsymbol{CD}$ is the reciprocal complementary distance matrix.[15]

For a symmetric $n \times n$ molecular matrix $\boldsymbol{M} = \boldsymbol{M}(G)$, whose (i,j)-entry is $\boldsymbol{M}_{ij}$, where $i,j = 1,2,\ldots,n$, let $M_i = \sum_{j=1}^{n} \boldsymbol{M}_{ij}$ be the sum of the entries in row i of $\boldsymbol{M}$. The Wiener operator of G and $\boldsymbol{M}$ is defined as $W(\boldsymbol{M},G) = \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} \boldsymbol{M}_{ij} = \sum_{i<j} \boldsymbol{M}_{ij}$.[22] If $M_i > 0$ for $i = 1,2,\ldots,n$, then the Ivanciuc-Balaban operator of G and $\boldsymbol{M}$ is defined as[23] $J(\boldsymbol{M},G) = \dfrac{m}{\mu+1}\sum_{v_i v_j \in E(G)} \left(M_i \cdot M_j\right)^{-1/2}$, where m is the number of edges and μ is the cyclomatic number of G. Let $\lambda_1(\boldsymbol{M},G), \lambda_2(\boldsymbol{M},G), \ldots, \lambda_n(\boldsymbol{M},G)$ be the eigenvalues of $\boldsymbol{M}$ arranged in non-increasing order.

Some of these matrices are computationally rather involved, especially for larger systems. Among the matrices listed above, the computationally-difficult matrices are the distance matrix, the detour matrix and the resistance-distance matrix. However, algorithms and computer programs for their computation do exist: Müller *et al.*[24] produced an program for computing the distance matrix, Rücker and Rücker[25] introduced a symmetry-based computation of the detour matrix and Babić *et al.*[26] presented a computational algorithm for obtaining the resistance-distance matrix.

It should be noted that in our exposition we use the terminology and apparatus of (chemical) graph theory.[8–10] Molecular graphs can be generated by replacing atoms and bonds with vertices and edges, respectively. Hydrogen atoms are usually neglected. A picture of a simple molecular graph G representing 1-ethylcyclopentane is given in Figure 1. In Table 1 we give examples of matrices presented in the text for the graph G from Figure 1, where $\boldsymbol{L}(G)$ is the Laplacian matrix, defined below.

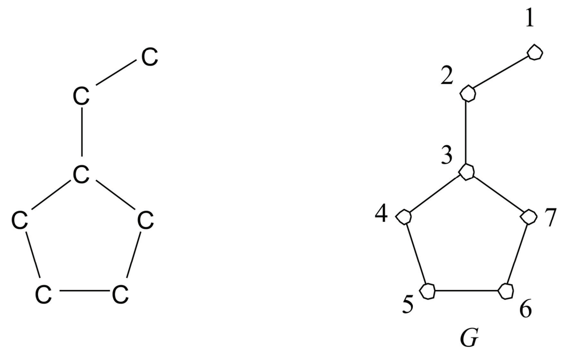

Figure 1. Carbon skeleton of 1-ethylcyclopentane and the corresponding labeled molecular graph *G*.

BASIC CONCEPTS AND NOTATIONS

Let G be a connected (molecular) graph. For $v_i \in V(G)$, the degree of v_i in G, denoted by δ_i, is the number of (first) neighbors of v_i. A graph is regular if every vertex has the same degree.[8] The term $\sum_{i=1}^{n}\delta_i^2$ is known as the first Zagreb index of G, denoted by $Zg(G)$.[27–30] It can be obtained by summing up the elements of the squared adjacency matrix $\boldsymbol{A}^2$. For the properties of the largest eigenvalue of the adjacency matrix $\lambda_1(\boldsymbol{A},G)$, see Ref. 11. The Laplacian matrix of G is $\boldsymbol{L} = \boldsymbol{L}(G) = \deg(G) - \boldsymbol{A}(G)$, where $\deg(G) = \mathrm{diag}(\delta_1, \delta_2, \ldots, \delta_n)$.[1]

Let P_n, S_n and K_n be, respectively, the path, the star and the complete graph with n vertices. Note that a path is a tree with two vertices of degree one and all the other vertices of degree two, a star is a tree with one vertex being adjacent to all the other vertices, and a complete graph is a simple graph in which every pair of distinct vertices is adjacent.[8] A bipartite graph G is a graph whose vertex-set V can be partitioned into two subsets V_1 and V_2 such that every edge of G connects a vertex in V_1 and a vertex in V_2.[8] Let $K_{a,b}$ be the complete bipartite graph with a vertices in one vertex-class and b vertices in the other vertex-class. Examples of P_n, S_n and K_n for $n = 6$ are depicted in Figure 2 and an example of $K_{a,b}$ for a = 3 and $b = 4$ is given in Figure 3.

The matching number of the graph G, denoted by $\beta(G)$, is the number of edges of a maximum matching. In chemistry, a perfect matching (a maximum matching with $\frac{n}{2}$ edges) is known as a Kekulé structure.[31] For a

Table 1. Examples of matrices presented in the text for the graph *G* given in Figure 1

$$\boldsymbol{A}(G)=\begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 \end{pmatrix}$$

$$\boldsymbol{D}(G)=\begin{pmatrix} 0 & 1 & 2 & 3 & 4 & 4 & 3 \\ 1 & 0 & 1 & 2 & 3 & 3 & 2 \\ 2 & 1 & 0 & 1 & 2 & 2 & 1 \\ 3 & 2 & 1 & 0 & 1 & 2 & 2 \\ 4 & 3 & 2 & 1 & 0 & 1 & 2 \\ 4 & 3 & 2 & 2 & 1 & 0 & 1 \\ 3 & 2 & 1 & 2 & 2 & 1 & 0 \end{pmatrix}$$

$$\boldsymbol{RW}(G)=\begin{pmatrix} 0 & 3 & 2 & 1 & 0 & 0 & 1 \\ 3 & 0 & 3 & 2 & 1 & 1 & 2 \\ 2 & 3 & 0 & 3 & 2 & 2 & 3 \\ 1 & 2 & 3 & 0 & 3 & 2 & 2 \\ 0 & 1 & 2 & 3 & 0 & 3 & 2 \\ 0 & 1 & 2 & 2 & 3 & 0 & 3 \\ 1 & 2 & 3 & 2 & 2 & 3 & 0 \end{pmatrix}$$

$$\boldsymbol{CD}(G)=\begin{pmatrix} 0 & 4 & 3 & 2 & 1 & 1 & 2 \\ 4 & 0 & 4 & 3 & 2 & 2 & 3 \\ 3 & 4 & 0 & 4 & 3 & 3 & 4 \\ 2 & 3 & 4 & 0 & 4 & 3 & 3 \\ 1 & 2 & 3 & 4 & 0 & 4 & 3 \\ 1 & 2 & 3 & 3 & 4 & 0 & 4 \\ 2 & 3 & 4 & 3 & 3 & 4 & 0 \end{pmatrix}$$

$$\boldsymbol{R}(G)=\begin{pmatrix} 0 & 1 & 2 & 14/5 & 16/5 & 16/5 & 14/5 \\ 1 & 0 & 1 & 9/5 & 11/5 & 11/5 & 9/5 \\ 2 & 1 & 0 & 4/5 & 6/5 & 6/5 & 4/5 \\ 14/5 & 9/5 & 4/5 & 0 & 4/5 & 6/5 & 6/5 \\ 16/5 & 11/5 & 6/5 & 4/5 & 0 & 4/5 & 6/5 \\ 16/5 & 11/5 & 6/5 & 6/5 & 4/5 & 0 & 4/5 \\ 14/5 & 9/5 & 4/5 & 6/5 & 6/5 & 4/5 & 0 \end{pmatrix}$$

$$\boldsymbol{DM}(G)=\begin{pmatrix} 0 & 1 & 2 & 6 & 5 & 5 & 6 \\ 1 & 0 & 1 & 5 & 4 & 4 & 5 \\ 2 & 1 & 0 & 4 & 3 & 3 & 4 \\ 6 & 5 & 4 & 0 & 4 & 3 & 3 \\ 5 & 4 & 3 & 4 & 0 & 4 & 3 \\ 5 & 4 & 3 & 3 & 4 & 0 & 4 \\ 6 & 5 & 4 & 3 & 3 & 4 & 0 \end{pmatrix}$$

$$\boldsymbol{RD}(G)=\begin{pmatrix} 0 & 1 & 1/2 & 1/3 & 1/4 & 1/4 & 1/3 \\ 1 & 0 & 1 & 1/2 & 1/3 & 1/3 & 1/2 \\ 1/2 & 1 & 0 & 1 & 1/2 & 1/2 & 1 \\ 1/3 & 1/2 & 1 & 0 & 1 & 1/2 & 1/2 \\ 1/4 & 1/3 & 1/2 & 1 & 0 & 1 & 1/2 \\ 1/4 & 1/3 & 1/2 & 1/2 & 1 & 0 & 1 \\ 1/3 & 1/2 & 1 & 1/2 & 1/2 & 1 & 0 \end{pmatrix}$$

$$\boldsymbol{RRW}(G)=\begin{pmatrix} 0 & 1/3 & 1/2 & 1 & 0 & 0 & 1 \\ 1/3 & 0 & 1/3 & 1/2 & 1 & 1 & 1/2 \\ 1/2 & 1/3 & 0 & 1/3 & 1/2 & 1/2 & 1/3 \\ 1 & 1/2 & 1/3 & 0 & 1/3 & 1/2 & 1/2 \\ 0 & 1 & 1/2 & 1/3 & 0 & 1/3 & 1/2 \\ 0 & 1 & 1/2 & 1/2 & 1/3 & 0 & 1/3 \\ 1 & 1/2 & 1/3 & 1/2 & 1/2 & 1/3 & 0 \end{pmatrix}$$

$$\boldsymbol{RCD}(G)=\begin{pmatrix} 0 & 1/4 & 1/3 & 1/2 & 1 & 1 & 1/2 \\ 1/4 & 0 & 1/4 & 1/3 & 1/2 & 1/2 & 1/3 \\ 1/3 & 1/4 & 0 & 1/4 & 1/3 & 1/3 & 1/4 \\ 1/2 & 1/3 & 1/4 & 0 & 1/4 & 1/3 & 1/3 \\ 1 & 1/2 & 1/3 & 1/4 & 0 & 1/4 & 1/3 \\ 1 & 1/2 & 1/3 & 1/3 & 1/4 & 0 & 1/4 \\ 1/2 & 1/3 & 1/4 & 1/3 & 1/3 & 1/4 & 0 \end{pmatrix}$$

$$\boldsymbol{L}(G)=\begin{pmatrix} 1 & -1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 3 & -1 & 0 & 0 & -1 \\ 0 & 0 & -1 & 2 & -1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 0 & 0 & -1 & 2 \end{pmatrix}$$

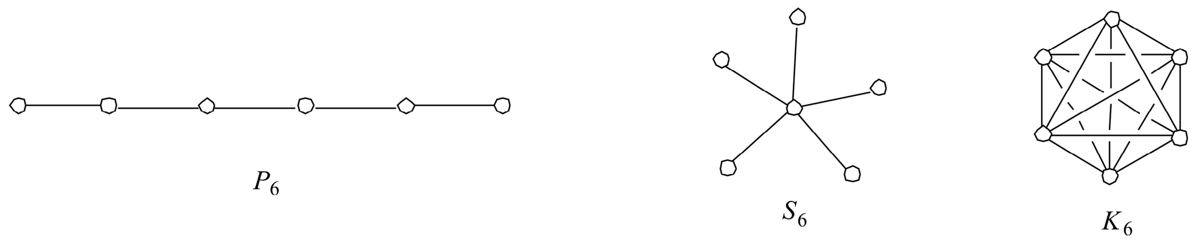

Figure 2. Examples of the path (P_6), star (S_6) and complete graph (K_6) on six vertices.

connected graph G with $n \geq 2$ vertices, $\beta(G) = 1$ if and only if $G = S_n$ or $G = K_3$.

A tree whose edges are some edges of a graph G and whose vertices are all of the vertices of the graph G is called a spanning tree of G.[8]

Let $\overline{G}$ be the complement of the graph G. The complement $\overline{G}$ of G is the simple graph which has $V(G)$ as its vertex-set and in which two vertices are adjacent if and only if they are not adjacent in G.[8] An example of a graph G and its complement $\overline{G}$ on five vertices is given in Figure 4.

WIENER-LIKE INDICES

$W(G) = W(\boldsymbol{D}, G)$ is the Wiener index[32,33] of the graph G. This is the oldest molecular descriptor, being in use since 1947.[32] Its mathematical properties and its use in QSPR and QSAR can be found in many sources, *e.g.*, Refs. 2–7,32–42.

In this section, we give results on six types of Wiener-like indices: the reverse Wiener index, the Harary index, the reciprocal reverse Wiener index, the reciprocal complementary Wiener index, the Kirchhoff index and the detour index. These molecular descriptors are of more recent date, but nevertheless found considerable use in QSPR and QSAR.[2]

Reverse Wiener index

First we consider the reverse Wiener index. The reverse Wiener index[14] of the graph G is defined as $\Lambda(G) = W(\boldsymbol{RW}, G) = \frac{1}{2}n(n-1)d - W(G)$. Note that the complementary Wiener index

$$W(\boldsymbol{CD}, G) = \frac{1}{2}n(n-1)(d+1) - W(G) = \Lambda(G) + \frac{1}{2}n(n-1)$$

has similar properties as $\Lambda(G)$. It was shown in Ref. 40 that for any tree T with n vertices, $\Lambda(S_n) \leq \Lambda(T) \leq \Lambda(P_n)$ with left (right, respectively) equality if and only if $T = S_n$ ($T = P_n$, respectively). Some results on the reverse Wiener index are summarized below.

Proposition 1.[43] Let G be a connected graph with $n \geq 2$ vertices. Then

$$0 \leq \Lambda(G) \leq \frac{n(n-1)(n-2)}{3}$$

with left (right, respectively) equality if and only if $G = K_n$ ($G = P_n$, respectively). Moreover, if G is a connected non-complete graph with m edges, then $\Lambda(G) \geq m$ with equality if and only if the diameter of G is 2.

Let $P_{n,d,i}$ be the tree formed from the path P_{d+1} whose vertices are labeled consecutively by $v_0, v_1, \ldots, v_d$ by attaching $n-d-1$ pendant vertices (vertices of degree one) to vertex v_i, where $1 \leq i \leq \left\lfloor \frac{d}{2} \right\rfloor$ and $2 \leq d \leq n-2$.

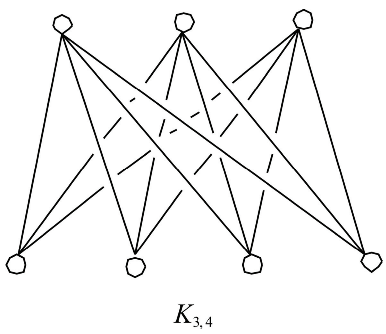

Figure 3. Example of the complete bipartite graph ($K_{3,4}$) on seven vertices.

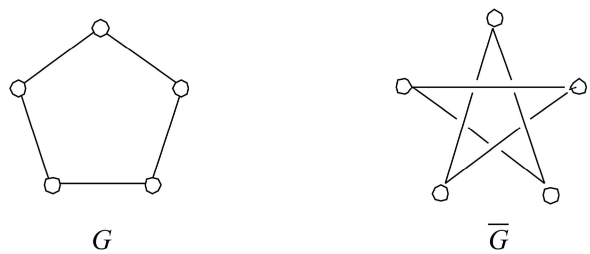

Figure 4. Example of the complement $\overline{G}$ of the graph G on five vertices.

Proposition 2.[43] Let T be a tree on n vertices with p pendant vertices or with the maximum degree p, where $3 \le p \le n-2$. Then $\Lambda(T) \le \Lambda\left(P_{n,n-p+1,\lfloor (n-p+1)/2 \rfloor}\right)$ with equality if and only if $T = P_{n,n-p+1,\lfloor (n-p+1)/2 \rfloor}$.

It should be noted that a tree T has an $(s, n-s)$-bipartition means as a bipartite graph the tree has s and $n-s$ vertices in its two vertex-classes, respectively.

Proposition 3.[43] Let T be a tree with n vertices. Suppose that either the matching number of T is s or T has an $(s, n-s)$-bipartition, where $2 \le s \le \left\lfloor \frac{n}{2} \right\rfloor$.

(i) If $s = \left\lfloor \frac{n}{2} \right\rfloor$, then $\Lambda(T) \le \Lambda(P_n)$ with equality if and only if $T = P_n$.

(ii) If $s \le \left\lfloor \frac{n}{2} \right\rfloor - 1$ and s is odd, then $\Lambda(T) \le \Lambda\left(P_{n,2s,s}\right)$ with equality if and only if $T = P_{n,2s,s}$.

(iii) If $s \le \left\lfloor \frac{n}{2} \right\rfloor - 1$ and s is even, then $\Lambda(T) \le \Lambda\left(P_{n,2s,s-1}\right)$ with equality if and only if $T = P_{n,2s,s-1}$.

Let $G_{n,i}$ be the graph formed from the path P_{n-1} whose vertices are labeled consecutively as $v_0, v_1, \ldots, v_{n-2}$ by adding a vertex v and edges vv_i and vv_{i+1}, where $0 \le i \le \left\lfloor \frac{n-3}{2} \right\rfloor$. Let $H_{n,i}$ be the graph formed from the path P_{n-1} by adding a vertex v and edges vv_i and vv_{i+2}, where $0 \le i \le \left\lfloor \frac{n-4}{2} \right\rfloor$. Let $L_{n,i}$ be the graph formed from the path P_{n-1} by adding a vertex v and edges vv_i, vv_{i+1} and vv_{i+2}, where $0 \le i \le \left\lfloor \frac{n-4}{2} \right\rfloor$. In Ref. 44, the n-vertex trees with the k-th largest reverse Wiener indices for all k up to $\left\lfloor \frac{n}{2} \right\rfloor + 1$, the n-vertex unicyclic graphs for all k up to $n-3$ or nearly to $n-3$, and the n-vertex bicyclic graphs for all k up to $\left\lfloor \frac{n-2}{2} \right\rfloor$ are determined. More precisely, we have:

Proposition 4.[44] Let G be a connected graph with $n \ge 5$ vertices.

(i) If G is a tree, then

$$\Lambda\left(P_{n,n-3,\lfloor (n-3)/2 \rfloor}\right) < \Lambda\left(P_{n,n-2,1}\right) < \Lambda\left(P_{n,n-2,2}\right) < \cdots < \Lambda\left(P_{n,n-2,\lfloor (n-2)/2 \rfloor}\right) < \Lambda\left(P_n\right)$$

and for any other n-vertex tree G, $\Lambda(G) < \Lambda\left(P_{n,n-3,\lfloor (n-3)/2 \rfloor}\right)$.

(ii) If G is a unicyclic graph, then the reverse Wiener indices of $G_{n,0}, G_{n,1}, \ldots, G_{n,\lfloor (n-3)/2 \rfloor}$ and $H_{n,0}, H_{n,1}, \ldots, H_{n,\lfloor (n-4)/2 \rfloor}$ may be ordered by

$$\Lambda\left(G_{n,0}\right) < \Lambda\left(G_{n,1}\right) < \cdots < \Lambda\left(G_{n,\lfloor (n-3)/2 \rfloor}\right),$$

$$\Lambda\left(H_{n,0}\right) < \Lambda\left(H_{n,1}\right) < \cdots < \Lambda\left(H_{n,\lfloor (n-4)/2 \rfloor}\right),$$

$$\Lambda\left(H_{n,\lfloor a_j \rfloor}\right) \le \Lambda\left(G_{n,j}\right) < \Lambda\left(H_{n,\lfloor a_j \rfloor + 1}\right), j = 1, 2, \ldots, \left\lfloor \frac{n-3}{2} \right\rfloor,$$

where left equality holds in above inequality if and only if $a_j = \frac{n-4-\sqrt{(n-2j)^2 - 4(n-3j)}}{2}$ is a nonnegative integer, and for any other n-vertex unicyclic graph G, $\Lambda(G) < \Lambda\left(G_{n,0}\right)$.

(iii) If G is a bicyclic graph, then

$$\Lambda\left(L_{n,0}\right) < \Lambda\left(L_{n,1}\right) < \cdots < \Lambda\left(L_{n,\lfloor (n-4)/2 \rfloor}\right)$$

and for any other n-vertex bicyclic graph G, $\Lambda(G) < \Lambda\left(L_{n,0}\right)$.

More results on the reverse Wiener index for trees, unicyclic graphs and bicyclic graphs may be found in Refs. 45−47.

Proposition 5.[43] Let G be a connected graph on $n \ge 5$ vertices with a connected $\overline{G}$. Then

$$\frac{n(n-1)}{2} \le \Lambda(G) + \Lambda(\overline{G}) \le \frac{(n-1)(n-2)(2n+3)}{6}$$

with left (right, respectively) equality if and only if both G and $\overline{G}$ have diameter 2 ($G = P_n$ or $G = \overline{P_n}$, respectively).

Harary index

The Harary index[2,19,20,48,49] of the graph G is defined as $H(G) = W(\boldsymbol{RD}, G)$. Gutman[50] noted that for any tree T with n vertices, $H(P_n) \le H(T) \le H(S_n)$ with left (right, respectively) equality if and only if $T = P_n$ ($T = S_n$, respectively). Note that the Harary index is even extended to disconnected graphs in measuring landscape connectivity.[51] Below we give some results for the Harary index.

Proposition 6.[49] Let G be a connected graph with $n \geq 2$ vertices and m edges. Then

$$H(P_n) + \frac{m-n+1}{2} \leq H(G) \leq \frac{n(n-1)}{4} + \frac{m}{2}$$

with left (right, respectively) equality if and only if $G = P_n$ or K_3 (G has diameter at most 2, respectively).

Proposition 7.[49] Let G be a triangle- and quadrangle-free connected graph with $n \geq 2$ vertices and m edges. Then

$$H(G) \leq \frac{n(n-1)}{6} + \frac{m}{2} + \frac{1}{12} Zg(G)$$

with equality if and only if G has diameter at most 3.

Proposition 8.[49] Let G be a triangle- and quadrangle-free connected graph with $n \geq 2$ vertices and m edges. Then

$$H(G) \leq \frac{n(n-1)}{4} + \frac{m}{2}$$

with equality if and only if G is the star or a Moore graph of diameter 2. (A Moore graph is a connected graph of diameter d and smallest cycle length $2d+1$. There are at most four Moore graphs of diameter 2: pentagon, Petersen graph, Hoffman-Singleton graph, and possibly a 57-regular graph with 3250 vertices whose existence is still an open problem.[10])

Proposition 9.[49] Let G be a connected graph on $n \geq 5$ vertices with a connected $\overline{G}$. Then

$$1 + \frac{(n-1)^2}{2} + n\sum_{k=2}^{n-1} \frac{1}{k} \leq H(G) + H(\overline{G}) \leq \frac{3n(n-1)}{4}$$

with left (right, respectively) equality if and only if $G = P_n$ or $G = \overline{P_n}$ (both G and $\overline{G}$ have diameter 2, respectively).

More results mainly on bounds for the Harary index may be found in Ref. 52 when the diameter is given.

Reciprocal reverse Wiener index

The reciprocal reverse Wiener index[21,53] of the graph G is defined as $R\Lambda(G) = W(\boldsymbol{RRW}, G)$.

Proposition 10.[53] Let G be a connected graph with $n \geq 3$ vertices. Then

$$0 \leq R\Lambda(G) \leq \frac{n(n-1)}{2} - 1$$

with left (right, respectively) equality if and only if $G = K_n$ ($G = K_n - e$, respectively), where $K_n - e$ is the graph obtained from the complete graph K_n by deleting an edge.

Proposition 11.[53] Let G be a connected graph with $n \geq 3$ vertices and m edges. Then

$$R\Lambda(G) \leq \begin{cases} m & \text{for } m \geq \frac{(n+1)(n-2)}{3} \\ \frac{n(n-1)}{2} - \frac{m}{2} - 1 & \text{for } m \leq \frac{(n+1)(n-2)}{3} \end{cases}$$

with equality if and only if G has diameter 2 for $m > \frac{(n+1)(n-2)}{3}$, G has diameter 3 and there is exactly one pair of vertices of distance 3 for $m < \frac{(n+1)(n-2)}{3}$, and either G has diameter 2 or G has diameter 3 and there is exactly one pair of vertices of distance 3 for $m = \frac{(n+1)(n-2)}{3}$.

Proposition 12.[53] Let G be a triangle- and quadrangle-free connected graph with n vertices, m edges and diameter $d \geq 3$. Then

$$R\Lambda(G) \leq \frac{n(n-1)}{2} - \frac{(d-2)m}{d-1} - \frac{d-3}{d-2}\left[\frac{1}{2} Zg(G) - m\right] - D(G,d)$$

with equality if and only if $d = 3, 4$.

Proposition 13.[53] Let G be a tree with $n \geq 4$ vertices. Then

$$n - 1 \leq R\Lambda(G) \leq \frac{n^2 - 4n + 7}{2}$$

with left (right, respectively) equality if and only if $G = S_n$ ($G = Y_n$, respectively), where Y_n is the tree formed by attaching a pendant vertex to a pendant vertex of the star S_{n-1}.

If G is a connected graph on $n \geq 5$ vertices with a connected complement $\overline{G}$, then $RA(G) + RA(\overline{G}) \leq \frac{2n^2 - 5n + 1}{2}$ with equality if and only if G is the graph formed from the path on 5 vertices by adding an edge between the two neighbors of its center. Moreover, if G and $\overline{G}$ have at most $\frac{(n+1)(n-2)}{3}$ edges, then $RA(G) + RA(\overline{G}) \leq \frac{3n^2 - 3n - 8}{4}$.[53]

Reciprocal complementary Wiener index

The reciprocal complementary Wiener index[20,54] of the graph G is defined as $RCW(G) = W(\boldsymbol{RCD}, G)$.

Proposition 14.[54] Let G be a non-complete connected graph with $n \geq 3$ vertices and m edges. Then

$$RCW(G) \leq \frac{n(n-1)}{2} - \frac{m}{2}$$

with equality if and only if G has diameter 2.

Proposition 15.[54] Let G be a connected graph with $n \geq 2$ vertices. Then

$$n - 1 \leq RCW(G) \leq \frac{n(n-1)}{2}$$

with left (right, respectively) equality if and only if $G = P_n$ ($G = K_n$, respectively). Moreover, if G is a non-complete connected graph with $n \geq 3$ vertices, then

$$RCW(G) \leq \frac{(n-1)^2}{2}$$

with equality if and only if $G = S_n$.

Proposition 16.[54] Let G be a triangle- and quadrangle-free connected graph with n vertices and m edges. If the diameter of G is at least 3, then

$$RCW(G) \leq \frac{n(n-1)}{2} - \frac{m}{6} - \frac{1}{4} Zg(G)$$

with equality if and only if G has diameter 3.

Proposition 17.[54] Let G be a connected graph on $n \geq 5$ vertices with a connected $\overline{G}$. Then

$$RCW(G) + RCW(\overline{G}) \leq \frac{3n(n-1)}{4}$$

with equality if and only if both G and $\overline{G}$ have diameter 2, whilst

$$RCW(G) + RCW(\overline{G}) \geq \begin{cases} \frac{n^2 + 5n - 6}{4} & \text{for } n \geq 9 \\ \frac{5n(n-1)}{12} + 1 & \text{for } 5 \leq n \leq 8 \end{cases}$$

with equality if and only if $G = P_n$ or $G = \overline{P_n}$ for $n \geq 9$, and both G and $\overline{G}$ have diameter 3 and exactly one pair of vertices of distance 3 for $5 \leq n \leq 8$.

Results on the first a few minimum reciprocal complementary indices of trees, unicyclic graphs and bicyclic graphs may be found in Ref. 55.

Kirchhoff index

The Kirchhoff index[16,26,56–61] of the graph G is defined as $Kf(G) = W(\boldsymbol{R}, G)$. It was proved in Ref. 16 that $\boldsymbol{R}_{ij} \leq \boldsymbol{D}_{ij}$ with equality if and only if there is exactly one path between v_i and v_j, and so $Kf(G) \leq W(G)$ with equality if and only if G is a tree. For a connected graph G with n vertices and m edges, Zhu *et al.*[62] and Gutman and Mohar[63] proved that $Kf(G) = n \sum_{i=1}^{n-1} \frac{1}{\lambda_i(\mathbf{L}, G)}$, and it was proved in Ref. 64 that $W(G) \leq (m - n + 2) Kf(G)$ with equality if and only if G is a tree. Palacios[65,66] produced closed formulas for some classes of graphs with symmetries. For a non-complete connected graph with $n \geq 3$ vertices, m edges and t spanning trees, Gutman *et al.*[67] derived lower and upper bounds for the Kirchhoff index as

$$n\left(\frac{1}{x_1} + \frac{n-2}{y_1}\right) \leq Kf(G) \leq n\left(\frac{n-2}{x_2} + \frac{1}{y_2}\right)$$

where $x_1 + (n-2)y_1 = 2m$, $x_1 y_1^{n-2} = nt$, $x_1 > y_1$; $(n-2)x_2 + y_2 = 2m$, $x_2^{n-2} y_2 = nt$, $x_2 > y_2$. Below we summarize some of our results for the Kirchhoff index.[60,61,68–70]

Proposition 18.[60] Let G be a connected graph with $n \geq 3$ vertices, m edges, maximum vertex degree Δ and t spanning trees. Then

$$Kf(G) \geq \frac{n}{1+\Delta} + \frac{n(n-2)^2}{2m - 1 - \Delta}$$

$$Kf(G) \geq \frac{n}{1+\Delta} + (n-2)n^{\frac{n-3}{n-2}}(1+\Delta)^{\frac{1}{n-2}} t^{-\frac{1}{n-2}}$$

with either equality if and only if $G = K_n$ or $G = S_n$.

Proposition 19.[60] Let G be a connected graph with $n \geq 2$ vertices. Then

$$Kf(G) \geq -1 + (n-1) \sum_{v_i \in V(G)} \frac{1}{\delta_i}.$$

The lower bound in Proposition 19 is attained if $G = K_n$ or $G = K_{t,n-t}$ for $1 \leq t \leq \left\lfloor \frac{n}{2} \right\rfloor$. A similar result as Proposition 19 is: if G is a connected graph with $n \geq 3$ vertices and $\delta_1 \geq \delta_2 \geq \cdots \geq \delta_n$, then $Kf(G) \geq n\left(\frac{1}{\delta_1+1} + \sum_{i=2}^{n-2} \frac{1}{\delta_i} + \frac{1}{\delta_{n-1}+\delta_n}\right)$ with equality if and only if $G = K_3$ or $G = S_n$.[70]

Proposition 20.[69] Let G be a connected bipartite graph with $n \geq 2$ vertices and maximum vertex degree Δ. Then

$$Kf(G) \geq \frac{n(2n-3)}{2\Delta}$$

with equality if and only if $G = K_{n/2,n/2}$.

Let G be a connected bipartite graph with $n \geq 2$ vertices and m edges. Let μ be the largest eigenvalue of the adjacency matrix of the line graph of G. From Ref. 11, we have $\mu \geq \frac{Zg(G)}{m} - 2$ with equality if and only if vertices in the same vertex-class of G have equal degree, where the lower bound is equal to the average degree of the line graph. From a relation between the characteristic polynomials of the Laplacian matrix of the (bipartite) graph G and the adjacency matrix of its line graph,[11] we have $\lambda_1(\boldsymbol{L}, G) = \mu + 2$. Then $\lambda_1(\boldsymbol{L}, G) \geq \frac{Zg(G)}{m}$ with equality if and only if vertices in the same partite set of G have equal degree. By the arguments in Ref. 68, we have

Proposition 21. Let G be a connected bipartite graph with $n \geq 3$ vertices, m edges and t spanning trees. Then

$$Kf(G) \geq n\left[\frac{m}{Zg(G)} + (n-2)\left(\frac{Zg(G)}{tnm}\right)^{\frac{1}{n-2}}\right],$$

$$Kf(G) \geq n\left[\frac{m}{Zg(G)} + \frac{(n-2)^2}{2m - \frac{Zg(G)}{m}}\right]$$

with either equality if and only if $G = K_{n/2,n/2}$.

For the bipartite graph G, we have by Cauchy-Schwarz inequality that $\lambda_1(\boldsymbol{L}, G) \geq 2\sqrt{\frac{Zg(G)}{n}}$ with equality if and only if G is regular. Then the bounds in previous proposition are better than the ones in Ref. 68:

$$Kf(G) \geq n\left[\frac{1}{2}\sqrt{\frac{n}{Zg(G)}} + (n-2)\left(\frac{2}{tn}\sqrt{\frac{Zg(G)}{n}}\right)^{\frac{1}{n-2}}\right],$$

$$Kf(G) \geq n\left[\frac{1}{2}\sqrt{\frac{n}{Zg(G)}} + \frac{(n-2)^2}{2m - 2\sqrt{\frac{Zg(G)}{n}}}\right].$$

The connectivity of a graph G is the minimum number of vertices whose removal from G yields a disconnected graph or a trivial graph (*i.e.* a graph consisting of a single vertex).[8] A coloring of a graph is an assignment of colors to its vertices such that any two adjacent vertices have different colors. The chromatic number of the graph G is the minimum number of colors in any coloring of G.[8]

Proposition 22.[60] Let G be a connected graph with $n \geq 2$ vertices and connectivity κ. Then

$$Kf(G) \geq n\left(\frac{\kappa}{n} + \frac{1}{\kappa} + 1 - \frac{\kappa+1}{n-1}\right)$$

with equality if and only if G is the graph obtained by adding κ edges between a vertex outside the complete graph K_{n-1} and vertices of K_{n-1}.

Proposition 23.[60] Let G be a connected graph with $n \geq 3$ vertices and chromatic number χ. Then

$$Kf(G) \geq n\left[\frac{\chi-1}{n} + \frac{(\chi-s)(r-1)}{n-r} + \frac{sr}{n-r-1}\right]$$

with equality if and only if G is the complete χ-partite graph with $\chi - s$ vertex classes of r vertices and s vertex classes of $r+1$ vertices, where r, s are integers with $n = r\chi + s$ and $0 \leq s < \chi$.

Proposition 24.[61] Let G be a connected graph with n vertices and matching number β, $2 \le \beta \le \left\lfloor \frac{n}{2} \right\rfloor$.

(i) If $\beta = \left\lfloor \frac{n}{2} \right\rfloor$, then $Kf(G) \ge n-1$ with equality if and only if $G = K_n$.

(ii) If $2 \le \beta \le \left\lfloor \frac{n}{2} \right\rfloor - 1$, then $Kf(G) \ge n\left(\frac{\beta}{n} + \frac{n-1}{\beta} - 1\right)$ with equality if and only if $G = K_\beta \vee \overline{K_{n-\beta}}$ (the graph formed by adding all possible edges from vertices of K_β to vertices of $\overline{K_{n-\beta}}$).

Proposition 25.[69] Let G be a connected graph with $n \ge 2$ vertices, maximum vertex degree Δ and minimum vertex degree δ. Then

$$\frac{n}{\Delta}\sum_{k=1}^{n-1}\frac{1}{\lambda_k(\mathcal{L},G)} \le Kf(G) \le \frac{n}{\delta}\sum_{k=1}^{n-1}\frac{1}{\lambda_k(\mathcal{L},G)}$$

with either equality if and only if G is regular, where $\mathcal{L}$ is the normalized Laplacian matrix of G defined by $\mathcal{L} = (\mathcal{L}_{ij})$ with $\mathcal{L}_{ij} = 1$ if $i = j$, $-\frac{1}{\sqrt{\delta_i \delta_j}}$ if v_i and v_j are adjacent, and 0 otherwise.[1,71,72]

Detour index

The detour index [17,73–75] of the graph G is defined as $\omega(G) = W(\boldsymbol{DM}, G)$. A graph is Hamilton-connected if each pair of distinct vertices are connected by a path containing all vertices of the graph.

Proposition 26.[76] Let G be a connected graph with $n \ge 3$ vertices. Then

$$(n-1)^2 \le \omega(G) \le \frac{n(n-1)^2}{2}$$

with left (right, respectively) equality if and only if $G = S_n$ (a Hamilton-connected graph, respectively).

Proposition 27.[76] Let G be a connected bipartite graph with $n \ge 2$ vertices. Then

$$\omega(G) \le \begin{cases} \frac{1}{2}(n-1)^3 & \text{if } n \text{ is odd} \\ \frac{1}{4}n(2n^2 - 5n + 4) & \text{if } n \text{ is even} \end{cases}$$

with equality if and only if $G = K_{\lfloor n/2 \rfloor, \lceil n/2 \rceil}$.

A number of results on the detour index for unicyclic graphs were given in Ref. 76, for example, the n-vertex unicyclic graphs with the first, the second and the third smallest and largest detour indices were determined.

EIGENVALUES

In this section, we consider the results on the eigenvalues, especially the largest eigenvalues of distance matrices.

Merris[77] obtained properties of the eigenvalues of distance matrix of a tree, in particular, for a tree T on $n \ge 2$ vertices. It was shown that

$$0 > \frac{-2}{\lambda_1(\boldsymbol{L},T)} \ge \lambda_2(\boldsymbol{D},T) \ge \frac{-2}{\lambda_2(\boldsymbol{L},T)} \ge \cdots \ge \frac{-2}{\lambda_{n-1}(\boldsymbol{L},T)} \ge \lambda_n(\boldsymbol{D},T),$$

which implies that the distance matrix of a tree T on $n \ge 2$ vertices has exactly one positive eigenvalue and $n-1$ negative eigenvalues. Ruzieh and Powers[78] showed that for any connected graph G with n vertices, $\lambda_1(\boldsymbol{D},G) \le \lambda_1(\boldsymbol{D},P_n) = \frac{1}{\cosh\theta - 1}$ with equality if and only if $G = P_n$, where θ is the positive solution of $\tanh\frac{\theta}{2}\tanh\frac{n\theta}{2} = \frac{1}{2}$, $\cosh x = \frac{e^x + e^{-x}}{2}$, $\tanh x = \frac{e^x - e^{-x}}{e^x + e^{-x}}$. Balaban *et al.*[79] proposed the use of the largest eigenvalue of the distance matrix as a structure-descriptor, which was successfully used to study the extent of branching and boiling points of alkanes.[80] Balasubramanian[81] computed the eigenvalues of the distance matrices of C_{20} - C_{90} fullerenes. Also, Gutman and Medeleanu[80] shown that for any tree T with n vertices and $S(\boldsymbol{D},T) = \sum_{i<j} \boldsymbol{D}_{ij}^2$,

$$\sqrt{\frac{1}{2}S(\boldsymbol{D},T) + n(n-1)\left(\frac{n-1}{4}\right)^{2/n}} < \lambda_1(\boldsymbol{D},T) < \sqrt{\frac{n-1}{2}S(\boldsymbol{D},T) + n\left(\frac{n-1}{4}\right)^{2/n}}.$$

Let G be a connected graph with $n \ge 3$ vertices and let $\boldsymbol{X}(G) = (\boldsymbol{X}_{ij}) = \left(\boldsymbol{L}(G) + \frac{1}{n}\boldsymbol{J}\right)^{-1}$, where $\boldsymbol{J}$ is the all 1's matrix. Note that $\sum_{i=1}^{n} \boldsymbol{X}_{ii} = 1 + \frac{Kf(G)}{n}$ (see Ref. 59). Then

$$\sum_{i=1}^{n} \boldsymbol{X}_{ii} + \sqrt{n\sum_{i=1}^{n} \boldsymbol{X}_{ii}^2} + \min\left\{-\frac{2}{\lambda_{n-1}(\boldsymbol{L},G)}, -2\right\} \leq$$
$$\leq \lambda_1(\boldsymbol{R},G) \leq \sum_{i=1}^{n} \mathbf{X}_{ii} + \sqrt{n\sum_{i=1}^{n} \boldsymbol{X}_{ii}^2 - \frac{2}{\lambda_1(\boldsymbol{L},G)}},$$

$$\sum_{i=1}^{n} \boldsymbol{X}_{ii} - \sqrt{n\sum_{i=1}^{n} \boldsymbol{X}_{ii}^2} + \min\left\{-\frac{2}{\lambda_{n-1}(\boldsymbol{L},G)}, -2\right\} \leq$$
$$\leq \lambda_n(\boldsymbol{R},G) \leq \sum_{i=1}^{n} \boldsymbol{X}_{ii} - \sqrt{n\sum_{i=1}^{n} \boldsymbol{X}_{ii}^2 - \frac{2}{\lambda_1(\boldsymbol{L},G)}}.$$

In the following, we give results on the eigenvalues (the largest and sometimes the smallest eigenvalues) of the distance matrices and some related matrices.[82–86] For a symmetric $n \times n$ molecular matrix $\boldsymbol{M} = \boldsymbol{M}(G)$, whose (i,j)-entry is $\boldsymbol{M}_{ij}$, where $i, j = 1, 2, \ldots, n$, let $S(\boldsymbol{M},G) = \sum_{i<j} \boldsymbol{M}_{ij}^2$. By the arguments and discussion in Refs. 83,84, and for $\lambda_n(\boldsymbol{M},G)$, using the inequalities $-\lambda_n(\boldsymbol{M},G) \leq \lambda_1(\boldsymbol{M},G)$ and $n^2\lambda_n(\boldsymbol{M},G)^2 \geq \sum_{i=1}^{n}\left[\lambda_i(\boldsymbol{M},G) - \lambda_n(\boldsymbol{M},G)\right]^2$, we have Propositions 28 and 29.

Proposition 28. Let G be a connected graph with $n \geq 2$ vertices and $\boldsymbol{M} = \boldsymbol{M}(G)$ a nonnegative symmetric $n \times n$ molecular matrix such that all diagonal entries are zero. Then

$$\lambda_1(\boldsymbol{M},G) \leq \sqrt{\frac{2(n-1)}{n} S(\boldsymbol{M},G)}$$

with equality for $\boldsymbol{M} = \boldsymbol{D}, \boldsymbol{R}$ (in Refs. 83,86) if and only if $G = K_n$. Moreover,

$$-\sqrt{\frac{2(n-1)}{n} S(\boldsymbol{M},G)} \leq \lambda_n(\boldsymbol{M},G) \leq -\sqrt{\frac{2S(\boldsymbol{M},G)}{n(n-1)}}$$

with left (right, respectively) equality for $\boldsymbol{M} = \boldsymbol{D}, \boldsymbol{R}$ (in Refs. 83,86) if and only if $G = K_2$ ($G = K_n$, respectively).

Proposition 29. Let G be a connected graph with $n \geq 2$ vertices and $\boldsymbol{M} = \boldsymbol{M}(G)$ a symmetric $n \times n$ molecular matrix whose diagonal entries are all zero. If $\boldsymbol{M}$ has exactly one positive eigenvalue (*e.g.*, $\boldsymbol{M} = \boldsymbol{R}$ in Ref. 59), then

$$\lambda_1(\boldsymbol{M},G) \geq \sqrt{S(\boldsymbol{M},G)}$$

with equality for $\boldsymbol{M} = \boldsymbol{D}$ of tree G (in Ref. 82) or $\boldsymbol{M} = \boldsymbol{R}$ (in Ref. 86) of any connected graph G if and only if $G = K_2$.

Let G be a connected graph with $n \geq 2$ vertices and $\boldsymbol{M} = \boldsymbol{M}(G)$ a nonnegative irreducible symmetric $n \times n$ molecular matrix such that all diagonal entries are zero. For any positive (column) vector $\boldsymbol{x} = (x_1, \ldots, x_n)^T$, we have $\lambda_1(\boldsymbol{M},G) \leq \max_{1\leq i\leq n} \frac{1}{x_i}\sum_{j=1}^{n} \boldsymbol{M}_{ij}x_j$ with equality if and only if $\boldsymbol{Mx} = \lambda_1(\boldsymbol{M},G)\boldsymbol{x}$ (see Ref. 87). On the other hand, since $\boldsymbol{M}$ is irreducible and symmetric, by Perron-Frobenius theorem, we have either $\lambda_1(\boldsymbol{M},G) > |\lambda_i(\boldsymbol{M},G)|$ for $i = 2, \ldots, n$ if $\boldsymbol{M}^2$ is irreducible or $\lambda_1(\boldsymbol{M},G) = -\lambda_n(\boldsymbol{M},G) > |\lambda_i(\boldsymbol{M},G)|$ for $i = 2, \ldots, n-1$ if $\boldsymbol{M}^2$ is reducible. For any vector $\boldsymbol{x} = (x_1, \ldots, x_n)^T \neq \mathbf{0}$, we have $\boldsymbol{x} = \sum_{i=1}^{n} c_i\boldsymbol{x}(i)$ where $\boldsymbol{x}(i)$, $i = 1, 2, \ldots, n$, are the orthonormal eigenvectors of $\boldsymbol{M}$ corresponding to $\lambda_i(\boldsymbol{M},G)$, and then

$$\frac{\boldsymbol{x}^T\boldsymbol{M}^2\boldsymbol{x}}{\boldsymbol{x}^T\boldsymbol{x}} = \frac{(\boldsymbol{Mx})^T\boldsymbol{Mx}}{\boldsymbol{x}^T\boldsymbol{x}} = \frac{\sum_{i=1}^{n} c_i^2\lambda_1(\boldsymbol{M},G)^2}{\sum_{i=1}^{n} c_i^2} \leq \lambda_1(\boldsymbol{M},G)^2$$

with equality if and only if $c_2 = \cdots = c_n = 0$ if $\boldsymbol{M}^2$ is irreducible, $\lambda_1(\boldsymbol{M},G) = -\lambda_n(\boldsymbol{M},G)$ and $c_2 = \cdots = c_{n-1} = 0$ if $\boldsymbol{M}^2$ is reducible, or equivalently, $\boldsymbol{M}^2\boldsymbol{x} = \lambda_1(\boldsymbol{M},G)^2\boldsymbol{x}$. By $\boldsymbol{x} = (M_1, \ldots, M_n)^T$ and $\boldsymbol{x} = (1, \ldots, 1)^T$ respectively in the inequalities above, and noting that if $\boldsymbol{M}^2\boldsymbol{x} = \lambda_1(\boldsymbol{M},G)^2\boldsymbol{x}$ for $\boldsymbol{x} = (1, \ldots, 1)^T$, then $\sum_{j=1}^{n} \boldsymbol{M}_{ij}M_j = \lambda_1(\boldsymbol{M}^2,G)$ for $i = 1, 2, \ldots, n$, and thus M_iM_j is a constant whenever $\boldsymbol{M}_{ij} > 0$, we have:[88,89]

Proposition 30. Let G be a connected graph with $n \geq 2$ vertices and $\boldsymbol{M} = \boldsymbol{M}(G)$ a nonnegative irreducible symmetric $n \times n$ molecular matrix. Then

$$\sqrt{\frac{\sum_{i=1}^{n} M_i^2}{n}} \leq \lambda_1(\boldsymbol{M},G) \leq \max_{1\leq i\leq n} \sum_{j=1}^{n} \boldsymbol{M}_{ij}\sqrt{\frac{M_j}{M_i}}$$

with either equality if and only if $M_1 = M_2 = \cdots = M_n$ if $\boldsymbol{M}^2$ is irreducible and there is a permutation matrix $\boldsymbol{Q}$ such that $\boldsymbol{Q}^{\mathrm{T}}\boldsymbol{MQ} = \begin{pmatrix} \mathbf{0} & \boldsymbol{B} \\ \boldsymbol{B}^{\mathrm{T}} & \mathbf{0} \end{pmatrix}$ where all the row sums of $\boldsymbol{B}$ are equal and all column sums of $\boldsymbol{B}$ are also equal if $\boldsymbol{M}^2$ is reducible.

$\boldsymbol{M} = \boldsymbol{D}, \boldsymbol{CD}, \boldsymbol{R}, \boldsymbol{DM}, \boldsymbol{RD}, \boldsymbol{RCD}$ for any connected graph satisfy the conditions in Proposition 30, and any bound is attained if and only if $M_1 = \cdots = M_n$ (the cases $\boldsymbol{M} = \boldsymbol{D}, \boldsymbol{RD}$ were treated in Refs. 83, 85). $\boldsymbol{M} = \boldsymbol{RW}, \boldsymbol{RRW}$ for any non-complete connected graph also satisfies the conditions in Proposition 30, and either bound is attained if and only if $M_1 = \cdots = M_n$ (equivalently, $D_1 = \cdots = D_n$ if $\boldsymbol{M} = \boldsymbol{RW}$) or G is a complete bipartite graph.[85] Recall that $D_i = \sum_{j=1}^{n} \boldsymbol{D}_{ij}$.

Using the Cauchy-Schwarz inequality to the left inequality in Proposition 30, we have:

Proposition 31. Let G be a connected graph with $n \geq 2$ vertices and $\boldsymbol{M} = \boldsymbol{M}(G)$ a nonnegative irreducible symmetric $n \times n$ molecular matrix such that all diagonal entries are zero. Then

$$\lambda_1(\boldsymbol{M}, G) \geq \frac{2W(\boldsymbol{M}, G)}{n}$$

with equality if and only if $M_1 = \cdots = M_n$.

$\boldsymbol{M} = \boldsymbol{D}, \boldsymbol{R}, \boldsymbol{CD}, \boldsymbol{RCD}, \boldsymbol{RW}, \boldsymbol{DM}$ for any connected graph G satisfy the conditions in Proposition 31 (For $\boldsymbol{M} = \boldsymbol{D}$, this has been noted in Ref. 90). Then from Proposition 31, lower bounds for $\lambda_1(\boldsymbol{M}, G)$ can easily be computed. Some examples follow:

(a) Let G be a connected graph with $n \geq 2$ vertices and m edges. Then $\lambda_1(\boldsymbol{D}, G) \geq 2(n-1) - \frac{2m}{n}$ with equality if and only if $G = K_n$ or G is a regular graph of diameter two. Moreover, if G is triangle- and quadrangle-free, then $\lambda_1(\boldsymbol{D}, G) \geq 3(n-1) - \frac{1}{n} Zg(\mathrm{G}) - \frac{2m}{n}$ with equality if and only if the row sums of $\boldsymbol{D}$ are all equal and the diameter of G is at most 3.[83]

(b) Let G be a connected graph with $n \geq 3$ vertices, m edges, t spanning trees and maximum vertex degree Δ. Then (by Proposition 18)

$$\lambda_1(\boldsymbol{R}, G) \geq \frac{2}{1+\Delta} + 2(n-2) n^{-\frac{1}{n-2}} (1+\Delta)^{\frac{1}{n-2}} t^{-\frac{1}{n-2}},$$

$$\lambda_1(\boldsymbol{R}, G) \geq \frac{2}{1+\Delta} + \frac{2(n-2)^2}{2m-1-\Delta}$$

with either equality if and only if $G = K_n$. By Proposition 19, and using the Cauchy-Schwarz inequality, $\lambda_1(\boldsymbol{R}, G) \geq \frac{n(n-1)}{m} - \frac{2}{n}$ and equality holds if $G = K_n$ or $G = K_{n/2,n/2}$.[86]

(c) Let G be a connected bipartite graph with $n \geq 3$ vertices, m edges, t spanning trees and maximum vertex degree Δ. Then (by Propositions 20 and 21)

$$\lambda_1(\boldsymbol{R}, G) \geq \frac{2n-3}{\Delta},$$

$$\lambda_1(\boldsymbol{R}, G) \geq \frac{2m}{Zg(G)} + 2(n-2)\left(\frac{Zg(G)}{tnm}\right)^{\frac{1}{n-2}}$$
$$\geq \sqrt{\frac{n}{Zg(G)}} + 2(n-2)\left(\frac{2}{tn}\sqrt{\frac{Zg(G)}{n}}\right)^{\frac{1}{n-2}},$$

$$\lambda_1(\boldsymbol{R}, G) \geq \frac{2m}{Zg(G)} + \frac{2m(n-2)^2}{2m^2 - Zg(G)}$$

with any equality if and only if $G = K_{n/2,n/2}$.[86]

Proposition 32.[84] Let G be a connected graph with $n \geq 2$ vertices. Suppose that $D_1 \geq \cdots \geq D_n$.

(i) If $D_1 > D_{n-k+1}$, $1 \leq k \leq n-1$, then

$$\lambda_1(\boldsymbol{D}, G) \leq \frac{D_1 - 1}{2} + \sqrt{\frac{(D_1+1)^2}{4} - k(D_1 - D_{n-k+1})}$$

with equality if and only if $k \leq n-2$, G is a graph with k vertices of degree $n-1$ and the remaining $n-k$ vertices have equal degree less than $n-1$.

(ii) If $D_l > D_n$, $1 \leq l \leq n-1$, then

$$\lambda_1(\boldsymbol{D}, G) > \frac{D_n - 1}{2} + \sqrt{\frac{(D_n+1)^2}{4} + l(D_l - D_n)}.$$

Proposition 33.[84] Let G be a connected graph with n vertices. Suppose that $DM_1 \geq \cdots \geq DM_n$.

(i) If $DM_1 > DM_{n-k+1}$, $1 \leq k \leq n-1$, then

$$\lambda_1(\boldsymbol{DM}, G) \leq \frac{DM_1 - 1}{2} + \sqrt{\frac{(DM_1+1)^2}{4} - k(DM_1 - DM_{n-k+1})}$$

with equality if and only if $k = 1$ and G is the star.

(ii) If $DM_l > DM_n$, $1 \leq l \leq n-1$, then

$$\lambda_1(\boldsymbol{DM}, G) > \frac{DM_n - 1}{2} + \sqrt{\frac{(DM_n+1)^2}{4} + l(DM_l - DM_n)}.$$

Proposition 34.[84] Let G be a connected graph with n vertices. Suppose that $RD_1 \geq \cdots \geq RD_n$.

(i) If $RD_1 > RD_{l+1}$, where $1 \leq l \leq n-1$, then

$$\lambda_1(\boldsymbol{RD},G) \le \frac{RD_{l+1}-1}{2} + \sqrt{\frac{(RD_{l+1}+1)^2}{4} + l(RD_1 - RD_{l+1})}$$

with equality if and only if $l \le n-2$, G is a graph with l vertices of degree $n-1$ and the remaining $n-l$ vertices have equal degree less than $n-1$.

(ii) If $RD_{n-k} > RD_n > k-1$, where $1 \le k \le n-1$, then

$$\lambda_1(\boldsymbol{RD},G) > \frac{RD_{n-k}-1}{2} + \sqrt{\frac{(RD_{n-k}+1)^2}{4} - k(RD_{n-k} - RD_n)}.$$

Proposition 35.[84] Let G be a connected graph with n vertices. Suppose that $CD_1 \ge \cdots \ge CD_n$.

(i) If $CD_1 > CD_{n-k+1}$, $1 \le k \le n-1$, then

$$\lambda_1(\boldsymbol{CD},G) < \frac{CD_1-1}{2} + \sqrt{\frac{(CD_1+1)^2}{4} - k(CD_1 - CD_{n-k+1})}.$$

(ii) If $CD_l > CD_n$, $1 \le l \le n-1$, then

$$\lambda_1(\boldsymbol{CD},G) > \frac{CD_n-1}{2} + \sqrt{\frac{(CD_n+1)^2}{4} + l(CD_l - CD_n)}.$$

Proposition 36.[86] Let G be a connected graph with $n \ge 3$ vertices. Then

$$\lambda_n(\boldsymbol{R},G) \le -\frac{2}{\lambda_{n-1}(\boldsymbol{L},G)}.$$

BALABAN-LIKE INDICES

Let G be a connected graph with $n \ge 2$ vertices. The $J(\boldsymbol{D},G)$ denotes the Balaban index of G,[91–93] which is a very useful molecular descriptor with attractive properties[2–7,10,94] and of high discriminatory power.[93] The computer program for computing the Balaban index of (molecular) graphs and weigthed graphs is also available.[95] $J(\boldsymbol{RD},G)$ is called the reciprocal Balaban index (also called the Harary-Balaban index[96] and the Harary-connectivity index[97]) of the graph G and $J(\boldsymbol{RW},G)$ the reverse Balaban index of the graph G.

The following proposition applies to the Balaban index ($\boldsymbol{M} = \boldsymbol{D}$), the reciprocal Balaban index ($\boldsymbol{M} = \boldsymbol{RD}$) for connected graphs, and the reverse Balaban index ($\boldsymbol{M} = \boldsymbol{RW}$) for non-complete connected graphs.[98,99] Let $\rho = \lambda_1(\boldsymbol{A},G)$. For the molecular matrix $\boldsymbol{M}$, let $\widetilde{M} = \max_{v_i \in V(G)} M_i$ and $\underline{M} = \min_{v_i \in V(G)} M_i$. For example, $\widetilde{D} = \max_{v_i \in V(G)} D_i$ and $\underline{D} = \min_{v_i \in V(G)} D_i$.

Proposition 37. Let G be a connected graph with n vertices and m edges and let $\boldsymbol{M}$ be a molecular matrix of G with positive row sums. Then

$$\frac{m^3}{(m-n+2)\rho W(\boldsymbol{M},G)} \le J(\boldsymbol{M},G) \le \le \frac{m\rho}{2(m-n+2)} \sum_{v_i \in V(G)} \frac{1}{M_i}$$

with left (right, respectively) equality if and only if G is either a regular graph such that M_i is a constant for every $v_i \in V(G)$ or a semiregular bipartite graph of degrees, say r_1, r_2 such that $r_1 / r_2 = M_i / M_j$ for any vertex v_i in the part with degree r_1 and any vertex v_j in the other part with degree r_2 ($\sum_{v_j v_i \in E(G)} M_j^{-1/2} = \rho M_i^{-1/2}$ for any $v_i \in V(G)$, respectively).

Let us first consider the Balaban index.

Proposition 38.[98] Let G be a connected graph with $n \ge 2$ vertices, m edges and minimum vertex degree δ.

(i) For $J(\boldsymbol{D},G)$,

$$\frac{m^3}{W(G)(m-n+2)\sqrt{2m-n+1}} \le J(\boldsymbol{D},G) \le \le \frac{mn}{2(m-n+2)(2n-2-\delta)}\rho$$

with left (right, respectively) equality if and only if G is the complete graph (G is a regular graph of diameter at most 2, respectively).

(ii) If the clique number is $k \ge 2$, then

$$\frac{m^2\sqrt{km}}{W(G)(m-n+2)\sqrt{2(k-1)}} \le J(\boldsymbol{D},G) \le \le \frac{mn}{2(m-n+2)(2n-2-\delta)}\sqrt{\frac{2(k-1)m}{k}}$$

with either equality if and only if G is a regular complete k-partite graph.

Proposition 39.[98] Let G be a connected graph with $n \ge 2$ vertices, m edges and maximum vertex degree Δ. Then

$$J(\boldsymbol{D},G) \le \frac{m}{2(m-n+2)}\left[\frac{n\Delta}{2n-2-\Delta} - \frac{\left(\sqrt{\widetilde{D}} - \sqrt{\underline{D}}\right)^2}{m\widetilde{D}\underline{D}}\right],$$

$$J(\boldsymbol{D},G) \le \frac{nm\Delta}{2(m-n+2)(2n-2-\Delta)}$$

with either equality if and only if G is a regular graph of diameter at most 2.

Let G be a connected graph with $n \ge 2$ vertices and m edges. Then by Proposition 39, $J(\boldsymbol{D},G) \le \frac{nm}{2(m-n+2)}$ with equality if and only if G is the complete graph.

Now we consider the reciprocal Balaban index.

Proposition 40.[99] Let G be a connected graph with $n \ge 2$ vertices and m edges. Then

$$\frac{m^3}{(m-n+2)\sqrt{2m-n+1}\ \mathrm{H}(G)} \le J(\boldsymbol{RD},G) \le \le \frac{m\sqrt{2m-n+1}}{2(m-n+2)} \sum_{v_i \in V(G)} \frac{1}{RD_i}$$

with either equality if and only if $G = K_n$. Also

$$J(\boldsymbol{RD},G) \ge \frac{2m^3}{n(n-1)(m-n+2)\sqrt{2m-n+1}}$$

with equality if and only if $G = K_n$.

Proposition 41.[99] Let G be a connected graph with $n \ge 2$ vertices, m edges, maximum vertex degree Δ, minimum vertex degree δ and diameter d. Then

$$J(\boldsymbol{RD},G) \le \frac{m}{2(m-n+2)} \left[\begin{array}{l} \min\left\{ \frac{nd\Delta}{n-1+(d-1)\Delta}, \frac{2md}{n-1+(d-1)\delta} \right\} \\ -\frac{\left(\sqrt{\widetilde{RD}}-\sqrt{\underline{RD}}\right)^2}{m\widetilde{RD}\,\underline{RD}} \end{array} \right],$$

$$J(\boldsymbol{RD},G) \le \frac{m}{2(m-n+2)} \min\left\{ \frac{nd\Delta}{n-1+(d-1)\Delta}, \frac{2md}{n-1+(d-1)\delta} \right\}$$

with either equality if and only if G is a regular graph and $d \le 2$.

Let G be a connected graph with $n \ge 2$ vertices and m edges. By Proposition 41, $J(\boldsymbol{RD},G) \le \frac{nm}{2(m-n+2)}$ with equality if and only if G is the complete graph.

Finally, we turn to the reverse Balaban index for non-completegraphs.

Proposition 42.[99] Let G be a non-complete connected graph with $n \ge 3$ vertices and m edges. Then

$$\frac{m^3}{(m-n+2)\sqrt{2m-n+1}\ \Lambda(G)} \le J(\boldsymbol{RW},G) < < \frac{m\sqrt{2m-n+1}}{2(m-n+2)} \sum_{v_i \in V(G)} \frac{1}{RW_i}$$

with left equality if and only if G is the star.

Theorem 43.[99] Let G be a connected graph with $n \ge 3$ vertices, m edges, maximum vertex degree Δ and diameter $d \ge 2$. Then

$$J(\boldsymbol{RW},G) \le \frac{m}{2(m-n+2)} \left[\frac{n}{d-1} - \frac{\left(\sqrt{\widetilde{RW}}-\sqrt{\underline{RW}}\right)^2}{m\widetilde{RW}\,\underline{RW}} \right],$$

$$J(\boldsymbol{RW},G) \le \frac{nm}{2(m-n+2)(d-1)}$$

with either equality if and only if G is a regular graph and $d = 2$.

Let G be a connected graph with $n \ge 3$ vertices, m edges, and $G \ne K_n$. By Proposition 43, $J(\boldsymbol{RW},G) \le \frac{nm}{2(m-n+2)}$ with equality if and only if G is a regular graph of diameter 2.

CONCLUDING REMARKS

In this report, we have surveyed mathematical properties, chiefly results for the upper and lower bounds, of molecular descriptors derived from a number of currently used distance matrices. The upper and lower bounds of a molecular descriptor are useful information since these data give the approximate range of the applicability of the descriptor in QSPR and QSAR in terms of structural parameters of a molecule (graph).

The distance matrices considered are the standard distance matrix ***D***, the reverse distance matrix or reverse Wiener matrix ***RW***, the reciprocal reverse Wiener matrix ***RRW***, the complementary distance matrix ***CD***, the resistance-distance matrix ***R***, the detour matrix ***DM***, the reciprocal distance matrix or Harary matrix ***RD*** and the reciprocal complementary distance matrix ***RCD***.

The distance-based molecular descriptors covered are the reverse Wiener index $W(\boldsymbol{RW},G)$, the complementary Wiener index $W(\boldsymbol{CD},G)$, the Harary index

W(***RD***,*G*), the reciprocal reverse Wiener index *W*(***RRW***,*G*), the reciprocal complementary Wiener index *W*(***RCD***,*G*), the Kirchhoff index *W*(***R***,*G*), the detour index *W*(***DM***,*G*), the Balaban index *J*(***D***,*G*), the reciprocal Balaban index or Harary-Balaban index *J*(***RD***,*G*) and the reverse Balaban index *J*(***RW***,*G*). Additionally, we also gave the bounds on the largest eigenvalues of the distance matrices.

Algorithms and software for computing most of these (and others not discussed here) molecular descriptors and setting the QSPR and QSAR models are summarized by Ivanciuc and Devillers.[100] Additionally, the strategy of setting up the optimum QSPR and QSAR models is also discussed by Mihalić and Trinajstić.[101] The ways of improving these models are presented by Lučić *et al*. in Ref. 102 and Amić *et al*. in Ref. 103.

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SAŽETAK

Matematička svojstva molekularnih deskriptora temeljenih na udaljenostima

Bo Zhou[a] i Nenad Trinajstić[b]

[a]*Department of Mathematics, South China Normal University, Guangzhou 510631, P. R. China*
[b]*Institut Ruđer Bošković, P. O. Box 180, HR-10002 Zagreb, Hrvatska*

Dan je pregled brojnih molekularnih deskriptora temeljenih na matricama udaljenosti i njihovim vlastitim vrijednostima. Razmatrane su sljedeće matrice udaljenosti: standardna matrica udaljenosti, obrnuta matrica udaljenosti, komplementarna matrica udaljenosti, matrica otpornih udaljenosti, matrica zaobilaznih udaljenosti, recipročna matrica udaljenosti i recipročna komplementarna matrica udaljenosti. Studirana su matematička svojstva sljedećih molekularnih deskriptora s naročitim naglaskom na njihove granične vrijednosti: obrnuti Wienerov indeks, Hararijev indeks, recipročni obrnuti Wienerov indeks, recipročni komplementarni Wienerov indeks, Kirchhoffov indeks, indeks zaobilaznih udaljenosti, Balabanov indeks, recipročni Balabanov indeks, obrnuti Balabanov indeks i najveća vlastita vrijednost matrica udaljenosti. Svi se navedeni molekularni deskriptori upotrebljavaju u modeliranju odnosa strukture, svojstava i aktivnosti.