Hindawi
Advances in Operations Research
Volume 2020, Article ID 3139867, 10 pages
https://doi.org/10.1155/2020/3139867

Research Article

Optimizing Wiener and Randić Indices of Graphs

A. C. Mahasinghe, K. K. W. H. Erandi, and S. S. N. Perera

Research & Development Center for Mathematical Modeling, Department of Mathematics, Faculty of Science, University of Colombo, Colombo 03, Sri Lanka

Correspondence should be addressed to A. C. Mahasinghe; anuradhamahasinghe@gmail.com

Received 9 June 2020; Accepted 4 August 2020; Published 26 September 2020

Academic Editor: Dylan F. Jones

Wiener and Randić indices have long been studied in chemical graph theory as connection strength measures of graphs. Later, these indices were used in different fields such as network analysis. We consider two optimization problems related to these indices, with potential applications to network theory, in particular to epidemiological networks. Given a connected graph and a fixed total edge weight, we investigate how individual weights must be assigned to edges, minimizing the connection strength of the graph. In order to measure the connection strength, we use the weighted Wiener index and a modified version of the ordinary Randić index. Wiener index optimization is linear, while Randić index optimization turns out to be both nonlinear and nonconvex. Hence, we adopt the technique of separable programming to generate solutions. We present our experimental results by applying relevant algorithms to several graphs.

1. Introduction

Topological indices of graphs have served as numerical invariants of chemical structures, characterizing the topology of the chemical structure graph theoretically. In most cases, these indices were used to measure the connection strength of chemical compounds. The first-ever such topological index found in the literature was the Wiener index, of which the intention was exploring thermodynamic and physiochemical properties of alkanes in terms of molecular shapes [1].Consequently, variants of the Wiener index and different other indices appeared for similar purposes, introducing a new field, chemical graph theory, into theoretical chemistry [2–4]. Though different indices intended for different characterizations of chemical compounds, they shared in common the notion of connection strength or compactness of the relevant graph structure.

Though these indices were originally confined to the chemical graph theory, their scope has later been extended as to include other subject areas as well. The applicability of topological indices to networks beyond chemical structures was initiated with the pioneering work by Gutman and Mohar in 1996, in which it was proven that a variant of the Wiener index coincides with the Kirchhoff index of electrical networks [5]. In 2002, Otte and Rousseau further extended the scope of topological indices by using them to analyze social networks [6]. In a recent work, Imran et al. analyzed interconnection networks using topological indices [7]. All these works used topological indices to characterize existing networks with fixed vertex and edge weights in order to derive information about the network. In contrast to this, Ghosh et al. investigated how the edge weights can be assigned subject to a fixed total weight, in order to optimize a topological index, together with an application into electrical circuits [8]. This application was interpreted as assigning resistors to the edges of an electric network, subject to a total fixed sum of resistance, aimed at minimizing the total effective resistance or, analogously, maximizing the connection strength. The topological measure for the total effective resistance has been taken as the algebraic connectivity (smallest nontrivial Laplacian eigenvalue) of the relevant graph, which is proven to be closely associated with the Wiener index [5]. Interestingly, the relevant optimization problem turns out to be convex, guaranteeing efficient solvability.

Optimizing topological indices subject to different constraints in different contexts has been the subject of interest in several previous works. Most of these optimization problems were related to the chemical graph theory, in particular to the design of chemical compounds. In [9], Raman and Maranas developed an integer programming model to optimize a combination of topological indices including Wiener and Randić indices and Kier's shape index [10]. Optimizing the molecular interconnectivity index for the design of polymers had been discussed in [11], with a solution scheme for the resulting nonconvex mixed-integer linear programming formulation. A computational scheme for designing new molecules in medicinal chemistry was described in [12] by Siddhaye et al., where the first-order molecular connectivity index was optimized through an integer programming reformulation and the branch-and-bound approach. An optimization problem of a different flavour in the context of chemical graph theory was considered in [13], where the simplex algorithm was used to derive optimal versions of several topological indices.

A few works on optimizing topological indices appear outside the realm of chemical graph theory as well. A concept paper by Preuß et al. [14] had proposed the optimization of Wiener and Randić indices to solve the maximum terrain coverage problem. A recent work [15] explored the possibility of optimizing the Wiener index for solving the critical node detection problem, where Benders algorithm [16] was adopted as the solution technique. An application of algebraic connectivity maximization to communication networks was discussed in [17].

The specific optimization problem considered by Ghosh et al. [8] is of particular interest and can be contrasted with the other optimization models with topological indices as the optimization is done subject to a constant edge weight sum. It is natural to seek what the nature of the problem would be if algebraic connectivity is replaced by a different topological index. Would that be an efficiently solvable optimization problem? Also, what if the objective was changed to minimizing the connection strength contrary to the electric network context? These are not merely questions of theoretical interest; there is a useful application to epidemiological networks. Consider the transmission of a vector-borne disease throughout a geographical region. This region can be considered as a network, of which the vertices represent cities or suburbs, while the edges represent their interconnections such as roads and channels, along which the vector-borne disease transmits [18]. The weight of an edge in this network could be regarded as a measure of favorable conditions for breeding sites of vectors. It has been claimed that the rapid transmission of such a disease is largely influenced by the compactness of the network [19, 20]. Thus, the health planners might be interested in minimizing the compactness of this network by eliminating the favorable conditions for vectors along the roads or water channels. However, this procedure is not without budgetary constraints. The total amount of budget available in the control process for eliminating vector breeding sites must be optimally utilized along the roads and channels. Thus, the total edge weight must be bounded by a constant. Whenever the aim is the minimization of the compactness of the epidemiological network, it is equivalent to optimizing an appropriate topological index subject to a fixed total edge weight. This is the main problem of interest in this work.

We first consider the Wiener index, which is the simplest topological index for characterizing the compactness of the network. However, in the context of epidemiological networks, a distance-based measure as Wiener index is less significant than a degree-based measure as a region with many interconnections is likely to contribute significantly to the spread of the disease. We find the degree-based topological index introduced by Randić in 1975 [21] ideal for our purpose. Though this was originally intended for measuring the extent of branching of the carbon atom in hydrocarbons, similar to the Wiener index, later developments of the Randić index have proven its applicability in different contexts [22–24].

Accordingly, we consider both Wiener index and Randić index to measure the compactness of the network in our optimization problem. The problem of optimizing the Wiener index turns out to be linear, thus trivially solvable. On the contrary, optimizing the Randić index is a challenging task as it turns out to be both nonlinear and nonconvex. In order to overcome the computational hardness, we adopt the technique of separable programming [25, 26] and replace respective nonlinear functions by their piecewise linear approximations, eventually ending up with an approximate solution to the problem.

The remainder of the paper is organized as follows. In Section 2, we reformulate the problem of minimizing the Wiener index of a graph subject to a fixed total edge weight as a linear program. In Section 3, we consider the same optimization problem by replacing the Wiener index with the Randić index, which turns out to be nonconvex. Our reformulation using separable programming techniques can be found in the same section. Section 4 contains our computational results, from which the discussion in Section 5 is motivated.

2. Optimizing the Wiener Index

The simplest and the pioneering topological index of graphs is the Wiener index. Consider a simple connected undirected graph $G(V, E)$ with n vertices. Then, the Wiener index $W(G)$ of a graph G is defined as

$$W(G) = \sum_{i=1}^{n} \sum_{j=1}^{n} \mathrm{dist}(i, j), \tag{1}$$

where $\mathrm{dist}(i, j)$ is the distance between ith and jth vertices of G. One may find several papers on finding Wiener indices of different graphs [27–29]. Though it is the unweighted version of the Wiener index which is used often, the vertex-weighted graph version was introduced later [30], which has achieved progress in the past few years [31, 32]. Furthermore, an edge-weighted version (known as the Gutman index) was introduced as a natural extension of the Wiener index [33]. We follow this as the edge-weighted Wiener index in our optimization problem. Accordingly, for a graph

G together with functions d and w, where d_i is the degree of the vertex i and w_{ij} is the weight of the edge (i, j), the weighted Wiener index is expressed as follows:

$$W_w(G) = \sum_{i=1}^{n} \sum_{(i,j)\in E} w_{ij} d_i d_j. \tag{2}$$

Our objective is minimizing the function $Z_1 = W_w(G)$ in equation (2), subject to relevant constraints. In terms of the epidemiological network context, the sole major constraint is the availability of budget for the control process. This constraint enforces that the allocation of resources to roads and channels must be done subject to a fixed total budget. Let the total (maximum possible) budget for resources be denoted by C. Then, the relevant constraint can be expressed as

$$\sum_{(i,j)\in E} w_{ij} \le C. \tag{3}$$

Finally, the nonnegativity of w_{ij} must be specified by

$$\forall (i, j) \in E, \quad w_{ij} \ge 0. \tag{4}$$

It can be seen that the optimization problem given by equations (2)–(4) is linear. Therefore, the solution is nontrivially obtained for Wiener index optimization.

3. Optimizing the Randić Index

The topological index introduced for characterizing the connection strength of chemical compounds by Milan Randić is widely known in chemical graph theory. This has been a subject of interest for graph theorists, and several works can be found on graph-theoretic aspects of the Randić index [34–36]. Being an elegant measure for the connection strength, this index has been applied in different contexts as well. Examples include measuring the robustness in cybernetics [22], reliability of communication networks [37], connectivity of mobile networks [38], and information content of a graph [39]. The ordinary Randić index is expressed as follows:

$$R(G) = \sum_{(i,j)\in E} \frac{1}{\sqrt{d(i)d(j)}}. \tag{5}$$

Clearly, Randić index is a degree-based topological index, unlike the distance-based Wiener index. Thus, unlike Wiener index optimization which was more into theoretical interest, Randić index optimization is directly relevant to our epidemiological application mentioned in Section 1. Moreover, a reduction of the Randić index results in the reduction of the Wiener index, a fact which can be seen by comparing equations (1) and (5) [40].

The edge-weighted version of the Randić index was introduced by Araujo and De la Peña as follows [41]:

$$R_w(G) = \frac{\left(\sum_{i=1}^{n} \sqrt{\sum_{(i,j)\in E} w_{ij}}\right)^2}{\sum_{i=1}^{n} \sum_{(i,j)\in E} w_{ij}}. \tag{6}$$

Aimed at minimizing the edge-weighted Randić index, now we express the objective function to be minimized as $Z_2 = R_w(G)$, subject to the same budgetary and nonnegativity constraints given by (3) and (4), respectively.

Thus, the problem turns out to be nonlinear. A closer look might reveal its nonconvexity. Recalling the problem of optimizing the topological index taken as algebraic connectivity turned out to be convex, a closed-form solution was obtained [8]. In contrast to this, optimizing the Randić index is a nonconvex optimization problem; thus, it is challenging to find the global optimum. Hence, instead of looking for closed-form exact solutions, we seek an approximate solution by using appropriate optimization and approximation schemes. It is not difficult to see that our objective function in equation (6) can be easily convertible to a form expressible as sums of functions of individual decision variables. This motivates us to make use separable programming technique for approximating the solution.

3.1. Separable Programming Formulation. The method of separable programming was first introduced for constrained optimization of nonlinear convex functions, whenever these functions are expressible as sums of functions of a single variable [25]. Functions with the latter mentioned property were called separable, and later works investigated the possibility of expanding the technique to nonconvex functions as well [42, 43]. Since its inception, separable programming has been a very useful optimization technique, with applications to several real problems including agricultural planning [44], linear complementarity problem [45], newsboy problem [46], and demand allocation [47].

Notice that the objective function in equation (6) is nonlinear and nonconvex. Hence, we convert the objective function to a separable form. Let

$$a_i = \sum_{j=1}^{n} w_{ij}. \tag{7}$$

From equation (6), our objective function can be restated as

$$Z_2 = \frac{\left(\sum_{i=1}^{n} \sqrt{a_i}\right)^2}{C} = \frac{1}{C}\left(\sum_{i=1}^{n} a_i + \sum_{i=1}^{n} \sum_{s=1}^{n} \sqrt{a_i a_s}\right). \tag{8}$$

Since $\sqrt{a_i} > 0$ for all $i \in \{1, 2, \ldots, n\}$, $\sqrt{a_i a_s}$ can be replaced by y_r, where $r \in \{1, 2, \ldots, n(n-1)/2\}$. Then, it is possible to transform the objective function to the separable form with the following constraint in the separable form:

$$\log(y_r) = \log\left(\sqrt{a_i}\right) + \log\left(\sqrt{a_s}\right). \tag{9}$$

Now, the objective function can be restated as

$$Z_2 = \frac{1}{C}\left(\sum_{i=1}^{n} a_i + 2 \sum_{r=1}^{((n(n-1))/2)} y_r\right). \tag{10}$$

This is to be minimized subject to

$$\sum_{i=1}^{n}\sum_{j\in V} w_{ij} \le C, \tag{11a}$$

$$a_i = \sum_{j=1}^{n} w_{ij}, \quad \forall i \in \{1,2,\ldots,n\}, \tag{11b}$$

$$\log(y_r) = \log\left(\sqrt{a_i}\right) + \log\left(\sqrt{a_s}\right), \quad \forall r \in \left\{\frac{1,2,\ldots,n(n-1)}{2}\right\}, \tag{11c}$$

$$w_{ij} \ge 0, \quad \forall i, j \in \{1,2,\ldots,n\}, \tag{11d}$$

$$a_i > 0, \quad \forall i \in \{1,2,\ldots,n\}, \tag{11e}$$

$$y_r > 0, \quad \forall r \in \left\{\frac{1,2,\ldots,n(n-1)}{2}\right\}. \tag{11f}$$

3.2. Linearly Approximated Program. Notice that the constraint given by equation (11c) is nonlinear. In order to approximate by piecewise linear functions, first, we restate equation (11c) as

$$g_{r1}(y_r) + \sum_{p=1}^{2} g_{r(1+p)}\left(x_p\right) = 0, \quad \forall r \in \left\{\frac{1,2,\ldots,n(n-1)}{2}\right\}, \tag{12}$$

where

$$g_{r1}(y_r) = \log y_r, \tag{13a}$$

$$g_{r2}(x_1) = -\log\sqrt{a_i}, \tag{13b}$$

$$g_{r3}(x_2) = -\log\sqrt{a_s}. \tag{13c}$$

Let the domain of $g_{r1}(y_r)$ be the interval $[C_0, C]$. Then, we divide the interval into m subdivisions of length d by defining α_{rk} as follows:

$$C_0 = \alpha_{r1} \le \alpha_{r2} \le \cdots \le \alpha_{rm} = C, \tag{14}$$

where

$$\left|\alpha_{rk} - \alpha_{r(k+1)}\right| = d. \tag{15}$$

Now, a point $y_r \in [C_0, C]$ can be uniquely expressed as

$$y_r = \lambda_{rk}\alpha_{rk} + \lambda_{r(k+1)}\alpha_{r(k+1)} = 1, \tag{16}$$

where

$$\lambda_{rk} + \lambda_{r(k+1)} = 1. \tag{17}$$

Then, the piecewise linear approximation to $g_{r1}(y_r)$ can be expressed as

$$g_{r1}(y_r) = \sum_{k=1}^{m} \lambda_{rk} g_{r1}(\alpha_{rk}), \tag{18}$$

where

$$\begin{aligned} y_r &= \sum_{k=1}^{m} \lambda_{rk}\alpha_{rk}, \\ \sum_{k=1}^{m} \lambda_{rk} &= 1. \end{aligned} \tag{19}$$

Let the domain of $g_{rp}(x_p)$ be the interval $[C_1, C]$. Then, we divide the interval into h subdivisions of length q by defining β_{pl} as follows:

$$C_0 = \beta_{p1} \le \beta_{p2} \le \cdots \le \beta_{ph} = C, \tag{20}$$

where

$$\left|\beta_{pl} - \beta_{p(l+1)}\right| = q. \tag{21}$$

Then, the piecewise linear approximation to $g_{rp}(x_p)$ can be expressed as

$$g_{rp}\left(x_p\right) = \sum_{l=1}^{h} \mu_{pl}\beta_{pl}, \tag{22}$$

where

$$\begin{aligned} x_p &= \sum_{l=1}^{h} \mu_{pl}\beta_{pl}, \\ \sum_{l=1}^{h} \mu_{pl} &= 1. \end{aligned} \tag{23}$$

Now, the nonlinear program is approximated by the following problem:

$$\text{minimize} \quad Z_3 = \frac{1}{C}\left(\sum_{r=1}^{((n(n-1))/2)} \sum_{k=1}^{m} \lambda_{rk}\alpha_{rk} + \sum_{i=1}^{n}\sum_{l=1}^{h} \mu_{il}\beta_{il}\right), \tag{24}$$

subject to

$$\sum_{i=1}^{n}\sum_{j\in V} w_{ij} \le C, \tag{25a}$$

$$\sum_{i=1}^{n}\sum_{l=1}^{h} \mu_{il}\beta_{il} = \sum_{(i,j)\in E} w_{ij}, \tag{25b}$$

$$\sum_{k=1}^{m} \lambda_{rk} g_{r1}(\alpha_{rk}) + \sum_{p=1}^{2}\sum_{l=1}^{h} \mu_{pl} g_{rp}(\beta_{pl}) = 0, \quad \forall r \in \left\{\frac{1,2,\ldots,n(n-1)}{2}\right\}, \tag{25c}$$

$$\sum_{k=1}^{m} \lambda_{rk} = 1, \quad \forall r \in \left\{\frac{1,2,\ldots,n(n-1)}{2}\right\}, \tag{25d}$$

$$\lambda_{rk}, \alpha_{rk} \ge 0, \quad \forall r \in \left\{\frac{1,2,\ldots,n(n-1)}{2}\right\}, \forall k \in \{1,2,\ldots,m,\} \tag{25e}$$

$$\sum_{l=1}^{h} \mu_{il} = 1, \quad \forall i \in \{1,2,\ldots,n\}, \tag{25f}$$

$$\mu_{il}, \beta_{il} \ge 0, \quad \forall i \in \{1,2,\ldots,n\}, \forall l \in \{1,2,\ldots,h\}, \tag{25g}$$

and at most two adjacent λ_{rk}'s are positive.

It can be seen that the linearly approximated problem given by equations (24) and (25) can be solved efficiently if the adjacency restriction is satisfied. Furthermore, it has been proven theoretically that if each individual function in the objective function is strictly convex and each individual function in constraints is convex for each relevant variable, then the solution of the linearly approximated formulation without the adjacency restriction is feasible to the original problem [26], which, however, is not the case with our problem given by equations (10) and (11). Several numerical techniques are available in the literature to overcome this issue and to find approximate solutions [42, 48–50]. We adopted the scheme given by Markowitz and Manne [50] to generate our computational results.

4. Computational Results

We implemented the algorithms using the mixed-integer programming model in SageMath. The experimentation took place over many graph structures up to 15 vertices. In particular, we tested all connected graphs up to 6 vertices. As for Wiener index optimization, despite the triviality of the formulation, some observations were of particular interest. For instance, the total weight was always assigned to a single edge of the graph. Furthermore, this edge always belonged to the edge dominating set of the graph (Table 1). This is quite natural, as the edges in the dominating set are the most significant in maintaining the connection strength of the graph, as each edge in the graph is either in the edge dominating set or adjacent to at least one edge in the edge dominating set. For instance, when the graph G_1 in Figure 1(a) was considered for Wiener index optimization, of which the results were derived making C in equation (3) equal to one, the optimal solution assigned a total weight of 1 to the edge $(1,4)$ in G_1. Interestingly, this edge alone makes an edge dominating set. It is easy to see that the vertex corresponding to $(1,4)$ in $L(G_1)$ as illustrated in Figure 2 makes a dominating set. Similarly, $(1,2)$ in G_2 (Figure 1(c)) and $(1,3)$ in G_3 (Figure 1(c)) were chosen which are the elements in dominating sets of their line graphs.

In contrast to this, in Randić index optimization, different weights were allocated to different edges. Therefore, it is natural to ask how Randić index optimization deals with the graph symmetries. In particular, it is important to see if the edge equivalences are considered when assigning weights. Therefore, we investigated the edge equivalences of these graphs to examine any possible connection to the optimal weighted assignment. Edge equivalence of graphs is defined under global symmetry relations of graphs, characterized in terms of edge automorphisms. This is defined in analogous to the notion of automorphisms in algebraic graph theory. The automorphism group of a graph G is the group formed by all structure-preserving permutations of its vertices and is denoted by $\mathrm{aut}(G)$. Two vertices u and v in G are said to be structurally equivalent if there is an automorphism σ in $\mathrm{aut}(G)$ such that $\sigma(u) = v$. Edge automorphism group of a graph G is defined as the automorphism group of the line graph $L(G)$ of G defined as the graph obtained by associating a vertex with each edge of G and connecting two vertices with an edge if the corresponding edges of G have a vertex in common. Thus, the edge set of a graph can be classified into equivalence classes, in the sense of global symmetry. The respective classification of the three graphs in Figure 1 can be seen in Figure 3.

Now, the question can thus be restated as follows: if two edges are structurally equivalent, does the optimal Randić index allocation assign equal weights to them? If yes, does it

Table 1: Optimal weight assignments for minimizing the Wiener index with edge dominating sets of graphs in Figure 1.

Graph	Nonzero weight assignment	Edge dominating set
G_1	$w(1,4) = 1$	$\{(1,4)\}$
G_2	$w(1,2) = 1$	$\{(1,2), (1,4)\}$
G_3	$w(1,3) = 1$	$\{(0,4), (1,3)\}$

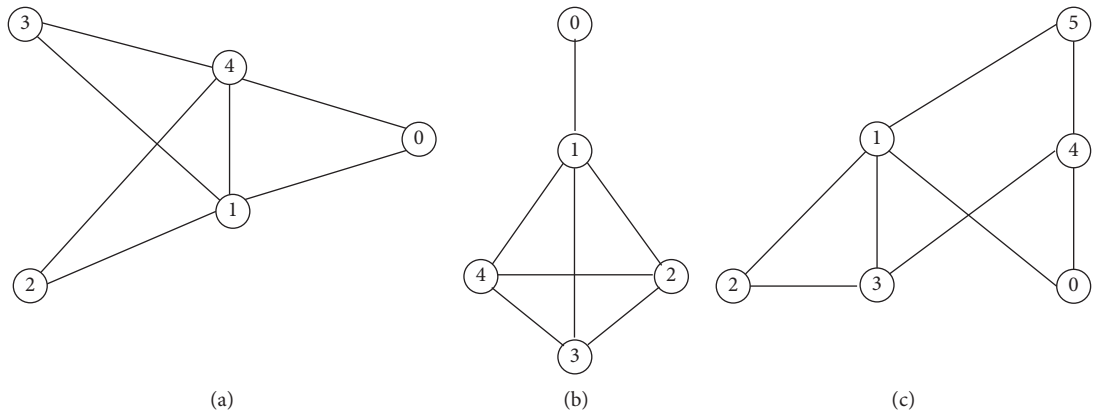


Figure 1: Three example graphs. (a) G_1. (b) G_2. (c) G_3.

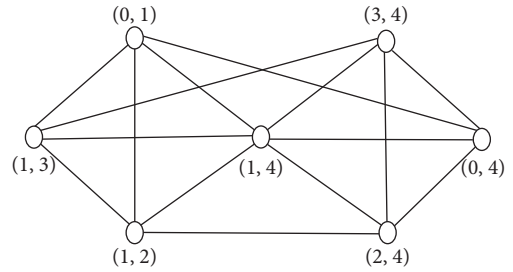


Figure 2: The line graph $L(G_1)$.

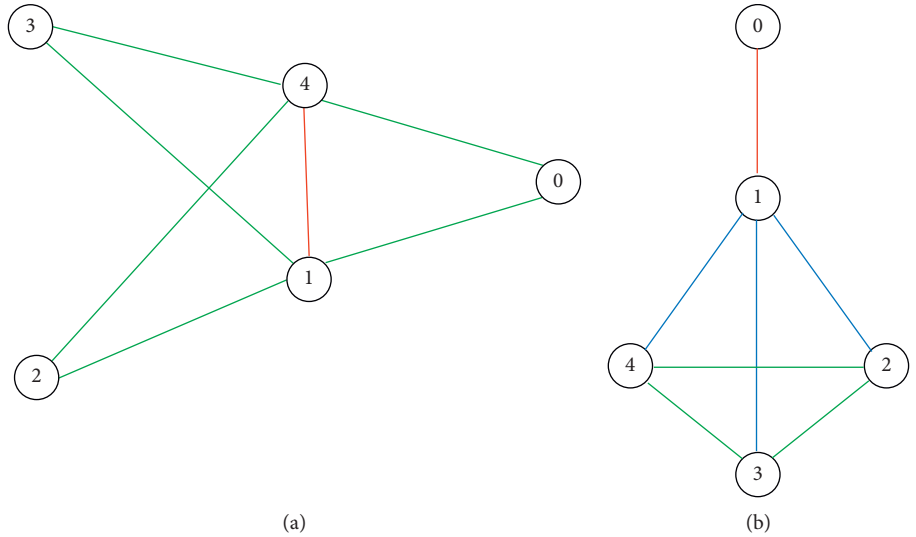
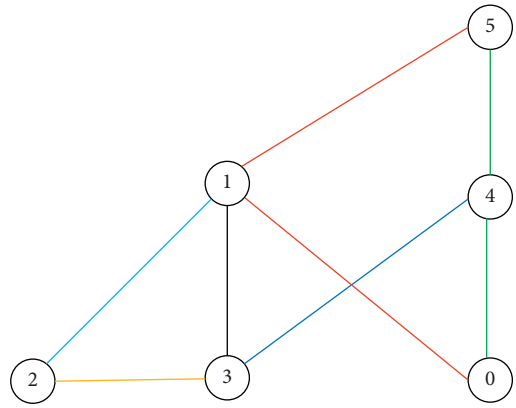


Figure 3: Continued.



(c)

Figure 3: Line graph of G_1 and classification of the edge sets into equivalence classes for the graphs in Figure 1. (a) G_1. (b) G_2. (c) G_3.

always distinguish two nonequivalent pairs of edges? The answers seemed to be negative. For instance, the edge automorphism group of G_1 is given by

$$\text{aut}\left(L\left(G_1\right)\right) = \{((1,2),(1,3))((2,4),(3,4)),((0,1),(0,4))((1,2),(2,4))((1,3),(3,4)),((0,1),(1,2))((0,4),(2,4))\}, \quad (26)$$

which implies that $(0,1)$ and $(0,4)$ are structurally equivalent edges, as illustrated in Figure 3(a). However, according to Table 2, they are allocated different weights. On the contrary, same weight has been assigned to $(1,2)$ and $(1,4)$, despite they belong to a different equivalence class. Therefore, it seems Randić index optimization does not reflect the global symmetry of a graph. Having said that, it must be mentioned that, during our experimentation, we encountered many graphs for which the Randić index optimization was perfectly harmonious with edge classification by equivalences. For instance, the three edge equivalence classes of G_2 (Figure 3(b)) are distinguished by the optimal allocation (Table 2), where each class is assigned its own weight unique to that class.

5. Discussion

Motivated by an epidemiological application and a previous work done by Ghosh et al. [8] related to electrical circuits, we considered the problem of assigning weights to edges of a graph, subject to a total fixed edge weight, with the aim of minimizing the connection strength of a graph, characterized first by the Wiener index and then by the Randić index. Though these two topological indices are closely related to each other, in particular, a change in the Randić index results in a change in the Wiener index, the two optimization problems of our consideration were far different from each other. Wiener index optimization was trivial, as it was a linear formulation, while Randić index optimization was a nonlinear and a nonconvex optimization problem. Therefore, we adopted the technique of separable programming to find approximate solutions to Randić index optimization. Finally, we presented our computational experience in the sense of dominating sets and global symmetry relations of a graph.

In a theoretical point of view, interesting comparisons can be made regarding optimizations of different topological indices. Recalling the optimization of the algebraic connectivity (first nontrivial Laplacian eigenvalue) is convex, one can compare Wiener index optimization, of which the solution procedure is much simpler, and Randić index optimization, of which it is harder. This may be extended further by considering optimization of different topological indices such as the Balaban index [51, 52], Harary index [53, 54], Graovac–Pisanski index [55], and Hosoya index [56]. On the contrary, it is interesting to investigate how these indices are related to the global symmetry of the graph. Although topological indices are studied extensively from graph-theoretic perspectives, their relation to automorphisms has not been paid much attention. It will be an interesting future work to consider if the optimal allocation of weights for other topological indices shows any relation with edge equivalences of graphs. It is noteworthy that a recent work introduced a variant of the Wiener index, moderated in light of global symmetry of graphs as characterized by the automorphism group [57]. It is natural to expect this version to resemble the global symmetry of the graph, of which the verification is left for future research studies. Furthermore, the relation of different topological indices to the edge dominating set could also be investigated.

In a practical point of view, different epidemiological conditions might require optimization of different topological indices. In the context of rapid transmission of a vector-borne disease, as our problem of interest, resources to control the disease must be assigned to edges

Table 2: Optimal weight assignment for minimizing Randić indices of graphs in Figure 1.

Graph	Weight
G_1	$w(0,1)=0, w(0,4)=0.2, w(1,2)=0, w(1,3)=0.2,$ $w(1,4)=0, w(2,4)=0.6, w(3,4)=0$
G_2	$w(0,1)=0.4, w(1,2)=0, w(1,3)=0, w(1,4)=0,$ $w(2,3)=0.2, w(2,4)=0.2, w(3,4)=0.2$
G_3	$w(0,1)=0, w(0,4)=0.25, w(1,2)=0, w(1,3)=0.125,$ $w(1,5)=0.25, w(2,3)0.3, w(3,4)=0.075, w(4,5)=0$

(interconnections). Instead, if it is a slowly propagating disease, resources may be allocated to vertices (regions), which could be restated as optimization of vertex-weighted versions of these indices, instead of the edge-weighted versions we have considered. In spite of the recent trend of intelligent resource allocation when controlling epidemics [58–61], only limited works are available in the mathematical and computational epidemiology literature on utilizing the resources optimally in order to minimize the transmission rate of the disease. Future research studies in this direction might be helpful for health planners, in particular in epidemic-prone countries where limitation of resources becomes a major obstacle to the control process.

Data Availability

The data used to support the findings of this study are included within the article.

Disclosure

The results in this manuscript were presented at the 8th International Eurasian Conference on Mathematical Sciences and Applications.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

Acknowledgments

This work was supported by grant RPHS/2016/D/05 of the National Science Foundation, Sri Lanka.

References

[1] H. Wiener, "Structural determination of paraffin boiling points," *Journal of the American Chemical Society*, vol. 69, no. 1, pp. 17–20, 1947.

[2] R. García-Domenech, J. Gálvez, J. V. de Julián-Ortiz, and L. Pogliani, "Some new trends in chemical graph theory," *Chemical Reviews*, vol. 108, no. 3, pp. 1127–1169, 2008.

[3] P. J. Hansen and P. C. Jurs, "Chemical applications of graph theory. part i. fundamentals and topological indices," *Journal of Chemical Education*, vol. 65, no. 7, p. 574, 1988.

[4] M. Randić, "On history of the randić index and emerging hostility toward chemical graph theory," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 59, pp. 5–124, 2008.

[5] I. Gutman and B. Mohar, "The quasi-wiener and the kirchhoff indices coincide," *Journal of Chemical Information and Computer Sciences*, vol. 36, no. 5, pp. 982–985, 1996.

[6] E. Otte and R. Rousseau, "Social network analysis: a powerful strategy, also for the information sciences," *Journal of Information Science*, vol. 28, no. 6, pp. 441–453, 2002.

[7] M. Imran, S. Hayat, and M. Y. H. Mailk, "On topological indices of certain interconnection networks," *Applied Mathematics and Computation*, vol. 244, pp. 936–951, 2014.

[8] A. Ghosh, S. Boyd, and A. Saberi, "Minimizing effective resistance of a graph," *SIAM Review*, vol. 50, no. 1, pp. 37–66, 2008.

[9] V. S. Raman and C. D. Maranas, "Optimization in product design with properties correlated with topological indices," *Computers & Chemical Engineering*, vol. 22, no. 6, pp. 747–763, 1998.

[10] L. B. Kier, "Indexes of molecular shape from chemical graphs," *Medicinal Research Reviews*, vol. 7, no. 4, pp. 417–440, 1987.

[11] K. V. Camarda and C. D. Maranas, "Optimization in polymer design using connectivity indices," *Industrial & Engineering Chemistry Research*, vol. 38, no. 5, pp. 1884–1892, 1999.

[12] S. Siddhaye, K. Camarda, M. Southard, and E. Topp, "Pharmaceutical product design using combinatorial optimization," *Computers & Chemical Engineering*, vol. 28, no. 3, pp. 425–434, 2004.

[13] A. R. Matamala and E. Estrada, "Generalised topological indices: optimisation methodology and physico-chemical interpretation," *Chemical Physics Letters*, vol. 410, no. 4-6, pp. 343–347, 2005.

[14] M. Preuß, M. Dehmer, S. Pickl, and A. Holzinger, "On terrain coverage optimization by using a network approach for universal graph-based data mining and knowledge discovery," in *Proceedings of International Conference on Brain Informatics and Health*, Springer, Berlin, Germany, pp. 564–573, August 2014.

[15] F. Hooshmand, F. Mirarabrazi, and S. A. MirHassani, "Efficient benders decomposition for distance-based critical node detection problem," *Omega*, vol. 93, Article ID 102037, 2020.

[16] J. F. Benders, "Partitioning procedures for solving mixed-variables programming problems," *Computational Management Science*, vol. 2, no. 1, pp. 3–19, 2005.

[17] H. Nagarajan, S. Rathinam, and S. Darbha, "On maximizing algebraic connectivity of networks for various engineering applications," in *Proceedings of 2015 European Control Conference (ECC)*, IEEE, Linz, Austria, pp. 1626–1632, July 2015.

[18] H. Saba, V. C. Vale, M. A. Moret, and J. G. V. Miranda, "Spatio-temporal correlation networks of dengue in the state of bahia," *BMC Public Health*, vol. 14, no. 1, p. 1085, 2014.

[19] L. Danon, A. P. Ford, T. House et al., "Networks and the epidemiology of infectious disease," *Interdisciplinary Perspectives Infectious Diseases*, vol. 2011, Article ID 284909, 708 pages, 2011.

[20] M. J. Keeling and K. T. D. Eames, "Networks and epidemic models," *Journal of The Royal Society Interface*, vol. 2, no. 4, pp. 295–307, 2005.

[21] M. Randić, "Characterization of molecular branching," *Journal of the American Chemical Society*, vol. 97, no. 23, pp. 6609–6615, 1975.

[22] P. De Meo, F. Messina, D. Rosaci, G. M. Sarné, and A. V. Vasilakos, "Estimating graph robustness through the randić index," *IEEE Transactions on Cybernetics*, vol. 48, no. 11, pp. 3232–3242, 2017.

[23] E. Estrada, "Randić index, irregularity and complex biomolecular networks," *Acta Chimica Slovenica*, vol. 57, no. 3, pp. 597–603, 2010.

[24] P. Riera-Fernandez, C. Munteanu, R. Martin-Romalde, A. Duardo-Sanchez, and H. Gonzalez-Diaz, "Markov-randic indices for QSPR Re-evaluation of metabolic, parasite- host, fasciolosis spreading, brain cortex and legal-social complex networks," *Current Bioinformatics*, vol. 8, no. 4, pp. 401–415, 2013.

[25] A. Charnes and C. E. Lemke, "Minimization of non-linear separable convex functionals," *Naval Research Logistics Quarterly*, vol. 1, no. 4, pp. 301–312, 1954.

[26] S. Sinha, *Mathematical Programming: Theory and Methods*, Elsevier, Amsterdam, Netherlands, 2005.

[27] M. Juvan, B. Mohar, A. Graovac, S. Klavzar, and J. Zerovnik, "Fast computation of the wiener index of fasciagraphs and rotagraphs," *Journal of Chemical Information and Modeling*, vol. 35, no. 5, pp. 834–840, 1995.

[28] P. Manuel, I. Rajasingh, B. Rajan, and R. S. Rajan, "A new approach to compute wiener index," *Journal of Computational and Theoretical Nanoscience*, vol. 10, no. 6, pp. 1515–1521, 2013.

[29] B. Mohar and T. Pisanski, "How to compute the wiener index of a graph," *Journal of Mathematical Chemistry*, vol. 2, no. 3, pp. 267–277, 1988.

[30] S. Klavžar and I. Gutman, "Wiener number of vertex-weighted graphs and a chemical application," *Discrete Applied Mathematics*, vol. 80, no. 1, pp. 73–81, 1997.

[31] T. Došlić, "Vertex-weighted wiener polynomials for composite graphs," *Ars Mathematica Contemporanea*, vol. 1, no. 1, pp. 66–80, 2008.

[32] W. Gao and W. Wang, "The vertex version of weighted wiener number for bicyclic molecular structures," *Computational and Mathematical Methods in Medicine*, vol. 2015, Article ID 418106, 10 pages, 2015.

[33] J. P. Mazorodze, S. Mukwembi, and T. Vetrík, "On the gutman index and minimum degree," *Discrete Applied Mathematics*, vol. 173, pp. 77–82, 2014.

[34] J. Gao and M. Lu, "On the randić index of unicyclic graphs," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 53, no. 2, pp. 377–384, 2005.

[35] Y. Hu, X. Li, and Y. Yuan, "Trees with minimum general randić index," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 52, pp. 119–128, 2004.

[36] M. Lu, L. Zhang, and F. Tian, "On the randić index of cacti," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 56, pp. 551–556, 2006.

[37] J. A. Rodríguez-Velázquez, A. Kamišalić, and J. Domingo-Ferrer, "On reliability indices of communication networks," *Computers & Mathematics with Applications*, vol. 58, no. 7, pp. 1433–1440, 2009.

[38] K. Kunavut and T. Sanguankotchakorn, "Qos routing for heterogeneous mobile ad hoc networks based on multiple exponents in the definition of the weighted connectivity index," in *Proceedings of 2011 Seventh International Conference on Signal Image Technology & Internet-Based Systems*, IEEE, Dijon, France, pp. 1–8, November 2011.

[39] I. Gutman, B. Furtula, and V. Katanić, "Randić index and information," *AKCE International Journal of Graphs and Combinatorics*, vol. 15, no. 3, pp. 307–312, 2018.

[40] D. Bonchev and N. Trinajstić, "Information theory, distance matrix, and molecular branching," *The Journal of Chemical Physics*, vol. 67, no. 10, pp. 4517–4533, 1977.

[41] O. Araujo and J. A. De la Peña, "Some bounds for the connectivity index of a chemical graph," *Journal of Chemical Information and Computer Sciences*, vol. 38, no. 5, pp. 827–831, 1998.

[42] J. H. Grotte, J. E. Falk, and P. F. McCoy, *A Computer Program for Solving Separable Non-Convex Optimization Problems*, Defense Technical Information Center, Fort Belvoir, VA, USA, 1978.

[43] H.-L. Li and C.-S. Yu, "A global optimization method for nonconvex separable programming problems," *European Journal of Operational Research*, vol. 117, no. 2, pp. 275–292, 1999.

[44] W. Thomas, L. Blakeslee, L. Rogers, and N. Whittlesey, "Separable programming for considering risk in farm planning," *American Journal of Agricultural Economics*, vol. 54, no. 2, pp. 260–266, 1972.

[45] J. F. Bard and J. E. Falk, "A separable programming approach to the linear complementarity problem," *Computers & Operations Research*, vol. 9, no. 2, pp. 153–159, 1982.

[46] L. L. Abdel-Malek and M. Otegbeye, "Separable programming/duality approach to solving the multi-product newsboy/gardener problem with linear constraints," *Applied Mathematical Modelling*, vol. 37, no. 6, pp. 4497–4508, 2013.

[47] A. Hassan and K. Abdelghany, "Dynamic origin-destination demand estimation using separable programming approach," *Advances in Transportation Studies*, vol. 43, 2017.

[48] M. S. Bazaraa, H. D. Sherali, and C. M. Shetty, *Nonlinear Programming: Theory and Algorithms*, John Wiley & Sons, Hoboken, NY, USA, 2013.

[49] G. B. Dantzig, "On the significance of solving linear programming problems with some integer variables," *Econometrica*, vol. 28, no. 1, pp. 30–44, 1960.

[50] H. M. Markowitz and A. S. Manne, "On the solution of discrete programming problems," *Econometrica*, vol. 25, no. 1, pp. 84–110, 1957.

[51] J. Devillers and A. Balaban, *Topological Indices and Related Descriptors in QSAR and QSPR*, Gordon Breach Scientific Publishers, London, UK, 1999.

[52] B. Zhou and N. Trinajstić, "Bounds on the balaban index," *Croatica Chemica Acta*, vol. 81, no. 2, pp. 319–323, 2008.

[53] B. Lučić, A. Miličević, S. Nikolić, and N. Trinajstić, "Harary index-twelve years later," *Croatica Chemica Acta*, vol. 75, no. 4, pp. 847–868, 2002.

[54] D. Plavšić, S. Nikolić, N. Trinajstić, and Z. Mihalić, "On the harary index for the characterization of chemical graphs," *Journal of Mathematical Chemistry*, vol. 12, no. 1, pp. 235–250, 1993.

[55] M. Hakimi-Nezhaad and M. Ghorbani, "On the graovac-pisanski index," *Kragujevac Journal of Science*, vol. 39, no. 1, pp. 91–98, 2017.

[56] H. Hosoya, "Topological index. a newly proposed quantity characterizing the topological nature of structural isomers of saturated hydrocarbons," *Bulletin of the Chemical Society of Japan*, vol. 44, no. 9, pp. 2332–2339, 1971.

[57] H. Shabani and A. R. Ashrafi, "Symmetry-moderated wiener index," *MATCH Communications in Mathematical and in Computer Chemistry*, vol. 76, pp. 3–18, 2016.

[58] Y. Deng, S. Shen, and Y. Vorobeychik, "Optimization methods for decision making in disease prevention and epidemic control," *Mathematical Biosciences*, vol. 246, no. 1, pp. 213–227, 2013.

[59] P. Kasaie, W. D. Kelton, A. Vaghefi, and S. J. Naini, "Toward optimal resource-allocation for control of epidemics: an agent-based-simulation approach," in *Proceedings of the 2010*

Winter Simulation Conference, IEEE, Baltimore, MD, USA, pp. 2237–2248, December 2010.

[60] V. M. Preciado, M. Zargham, C. Enyioha, A. Jadbabaie, and G. Pappas, "Optimal vaccine allocation to control epidemic outbreaks in arbitrary networks," in *Proceedings of 52nd IEEE Conference on Decision and Control*, IEEE, Florence, Italy, pp. 7486–7491, June 2013.

[61] G. S. Zaric and M. L. Brandeau, "Dynamic resource allocation for epidemic control in multiple populations," *Mathematical Medicine and Biology*, vol. 19, no. 4, pp. 235–255, 2002.