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On The Reliability Wiener Number[1]

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ABSTRACT. One of the generalizations of the Wiener number to weighted graphs is to assign probabilities to edges, meaning that in nonstatic conditions the edge is present only with some probability. The Reliability Wiener number is defined as the sum of reliabilities among pairs of vertices, where the reliability of a pair is the reliability of the most reliable path. Closed expressions are derived for the Reliability Wiener number of paths, cycles, stars and brooms. It is shown that the Reliability Wiener number can be used as a measure of branching.

Keywords: Reliability Wiener number, edge probability, branching.

1. INTRODUCTION

Distance is a basic yet very important notion in many applications of graph theory including mathematical chemistry and computer science [6, 7]. The sum of all distances, in mathematical chemistry well known as the Wiener number of a graph [21], is also studied in mathematics [14] and in computer science [3, 13, 4]. Until today, a remarkably large number of modifications and extensions of the Wiener number was put forward (see for example the special issues and books [6, 7, 8, 9]). However, there are relatively few studies of a seemingly natural extension of Wiener number where the meaning of the edge weights are probabilities. The reliability Wiener number studied here is a generalization of Wiener number that is proven to be relevant in the studies of interconnection and social networks [16, 2, 17]. We believe that it may be also of interest in chemical graph theory, because the idea to assign probabilities to edges is a natural model taking into account that in the

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structure observed there are some (or all) edges (bonds) that are not static. Various probabilities easily allow modelling different types of chemical bonds. In particular, chemical bonds are of different types and it is well-known that under certain conditions the bonds can break with certain probability. Another motivating example is the benzen ring where there are double bonds which form a perfect matching in the complete graph on 6 vertices. There are 10 possible perfect matchings among 6 vertices. Usually, only two matchings that are most probably based on the fixed embedding of the ring into the space are considered (so called Kekulé structures). However it also makes sense to take into accunt the extended pairings (Dewar, Claus and others) for a given connectivity as was done for example in [5]. Therefore, it may be natural to give certain probabilites to the matchings and thus to double bonds. For example, the two Kekulé structures may naturally be assumed to have probability 1/2 each, but there are other possiblities of course. As the definition we use here has first appeared in studying reliability of networks [16], we call the generalization of the Wiener number studied here the reliability Wiener number.

In this paper we study the reliability Wiener number defined as the sum of reliabilities among pairs of vertices, where the reliability of a pair is the reliability of the most reliable path. In the next section basic definitions are given. In Section 3, closed expressions are derived for the Reliability Wiener number of paths, cycles, stars and brooms. Finally, in Section 4, we show that the Reliability Wiener number can be used as a measure of branching.

2. DEFINITIONS

A *weighted graph* $G=(V,E,p)$ is a combinatorial object consisting of an arbitrary set $V=V(G)$ of *vertices*, a set $E=E(G)$ of unordered pairs $\{u,v\}=uv=e$ of distinct vertices of G called *edges*, and a *weighting function*, p. The weight function $p:E(G)\mapsto[0,1]$ is interpreted as the probability of edges. That is, $1-p(e)$ is the probability that edge $e\in E(G)$ breaks. Hence it is natural to assume that $p(e)>0$ for any edge of the graph (bond). Alternatively, we can consider the complete graph and model non existing edges by setting $p(e)=0$. As usual, the order and size of G are denoted by $\mathrm{n}=|\mathrm{V(G)}|$ and $m=|E(G)|$.

Note that in this model, the distance as is usually defined in graph theory is not considered. Instead of distance we have reliability of a connection and we only have paths that are more or less reliable. Of course, when the probabilities of edges are not very different, shorter paths will be much more reliable than longer paths. Hence the shortest paths (in terms of distance) are likely to contribute to the Reliability Wiener number. It is possible to extend the model and combine the two notions (reliability distance and classical distance) but we do not attempt to do it here.

We mention in passing that the results on weighted Wiener number as considered in [19] and related generalization of the Hosoya-Wiener polynomial [20] do not apply in the current context, because they regard weights (lengths) of paths as the sums of weights (lengths) of edges while here the weights (reliabilities) of paths are product of weights (probabilities) of edges.

A *path* P between u and v is a sequence of distinct vertices $u = v_i,\ v_{i+1},\ \ldots,\ v_{k-1},$ $v_k = v$ such that each pair $v_l v_{l+1}, (l = i,\ldots,k-1)$ is connected by an edge. The *length* $\ell(P)$ of a path P is the number of edges on P. The *distance* $d_G(u,v)$, or simpler $d(u,v)$, between vertices u and v in graph G is the length of a shortest path between u and v. If there is no such path, we write $d(u,v) = \infty$.

We can define the *reliability* of a path P with

$$p(P) = \prod_{l=i}^{k-1} p(v_l, v_{l+1}).$$

In the special case when all edges have probability 1, $p(P) = 1$ for any path P. Of course, several paths from one vertex to another can exist. The maximum reliability between two vertices is reached using the path with maximum reliability. In [16], the notion of *reliability of a graph* was introduced by a version of Wiener number where instead of the usual distance the most reliable path between each pair of vertices is considered. Following this idea, we define: For two vertices $u, v \in V(G)$ denote with $P_{\overrightarrow{uv}}$ the set of all directed paths from u to v. The weight of the most reliable path from u to v is called the *reliability of* (u,v):

$$F_{\overrightarrow{uv}} = \max_{P \in P_{\overrightarrow{uv}}} \{p(P)\}.$$

Furthermore, we set $F_{\overrightarrow{uu}} = 1$ for all $u \in V(G)$ and define

$$R^+(u) = \sum_{v \in V(G)-u} F_{\overrightarrow{uv}} \qquad \textit{the weighted out-reliability of vertex } u,$$

$$R^-(u) = \sum_{v \in V(G)-u} F_{\overrightarrow{vu}} \qquad \textit{the weighted in-reliability of vertex } u,$$

$$W_{R^+}(G) = \sum_{u \in V(G)} R^+(u) \qquad \textit{the out-reliability Wiener number of } G,$$

$$W_{R^-}(G) = \sum_{u \in V(G)} R^-(u) \qquad \textit{the in-reliability Wiener number of } G.$$

As undirected graphs are studied here, obviously, because $p(u,v) = p(v,u) = p(e)$ for any edge $e = \{u,v\}$ in G, $R^-(u) = R^+(u) =: R(u)$ and $W_{R^-}(G) = W_{R^+}(G)$, so we can define the *reliability Wiener number* by

$$W_R(G,p)=\frac{1}{2}\sum_{u\in V(G)}R(u)=\frac{1}{2}\sum_{u\in V(G)}\sum_{v\in V(G)}F_{\overrightarrow{uv}}=\frac{1}{2}\sum_{u\neq v}F_{\overrightarrow{uv}}. \tag{1}$$

The reliability Wiener number of G is a measure of the capacity of the vertices of G of transmitting information in a reliable form, where the information is transmitted through the most reliable path. As suggested in [16], the problem of finding $F_{\overleftarrow{uv}}$ can be solved by using Dijkstra's algorithm on a weighted digraph $G'=(V,E,-\ln p)$. Hence W_R can be computed efficiently.

3. PROPERTIES OF RELIABILITY WIENER NUMBER

In this section we derive closed expressions for the reliability Wiener number of paths, cycles, stars and brooms. We conclude the section by stating general lower and upper bounds for $W_R(G,p)$.

Proposition 1 *If $G=P_n$ is a path with n vertices $v_1,v_2,\ldots,v_n$ and $p_i = p(v_i,v_{i+1}), i=1,\ldots,n-1$, then*

$$W_R(P_n)=\sum_{i=1}^{n-1}p_i+\sum_{i=1}^{n-2}p_i\,p_{i+1}+\sum_{i=1}^{n-3}p_i\,p_{i+1}\,p_{i+2}+\cdots+p_1\,p_2\cdots p_{n-1}.$$

If $G=P_n$ is a path with n vertices and all link probabilities are equal, say $p(e)=p_0$ for all $e\in E(G)$, where $0<p_0<1$ is a constant, then

$$W_R(P_n)=(n-1)\frac{p_0}{1-p_0}-\left(\frac{p_0}{1-p_0}\right)^2(1-p_0^{n-1}).$$

Proof:

$$W_R(P_n)=\sum_{i=1}^{n-1}p_0+\sum_{i=1}^{n-2}p_0^2+\sum_{i=1}^{n-3}p_0^3+\cdots+p_0^{n-1}$$

$$=(n-1)p_0+(n-2)p_0^2+(n-3)p_0^3+\cdots+p_0^{n-1}$$

$$=\sum_{k=1}^{n-1}kp_0^{n-k}=\sum_{l=1}^{n-1}\sum_{k=1}^{n-l}p_0^k=\sum_{l=1}^{n-1}p_0\frac{1-p_0^{n-l}}{1-p_0}$$

$$=(n-1)\frac{p_0}{1-p_0}-\left(\frac{p_0}{1-p_0}\right)^2(1-p_0^{n-1}).$$

□

Remark. In the case when $p_0=1$:

$$W_R(P_n) = \sum_{k=1}^{n-1} k = \binom{n}{2}.$$

Proposition 2 *If* $G = C_n$ *is a cycle with* n *vertices* $v_1, v_2, ..., v_n$ *and* $\mathrm{p_i} = \mathrm{p(v_i, v_{i+1})}$, $\mathrm{i} = 1,...,\mathrm{n}-1$ *and* $p_n = p(v_n, v_1)$ *then*

$$W_R(C_n) = \sum_{i=1}^{n-1}\sum_{j=i+1}^{n} \max\{p_i p_{i+1} \cdots p_{j-1},\ p_{i-1}p_{i-2} \cdots p_{i-j+1}\},$$

with definition $p_k := p_{n+k}$ *for* $k \le 0$.

If all link probabilities are equal, $p(e) = p_0$ *for all* $e \in E(G)$, *where* $0 < p_0 < 1$ *is a constant, then*

$$W_R(C_n) = \begin{cases} np_0 \dfrac{1-p_0^{n/2}}{1-p_0} - \dfrac{n}{2} p_0^{n/2} & ; \quad n \text{ even}, \\ np_0 \dfrac{1-p_0^{(n-1)/2}}{1-p_0} & ; \quad n \text{ odd}. \end{cases}$$

Proof:

$$W_R(C_n) = \sum_{i=1}^{n-1}\sum_{j=i+1}^{n} \max\{p_0^{j-i},\ p_0^{n-j+i}\} = \sum_{i=1}^{n-1}\sum_{j=i+1}^{n} p_0^{\min\{j-i, n-j+i\}} =$$
$$= \sum_{i=1}^{n-1}\left(p_0^{\min\{1,n-1\}} + p_0^{\min\{2,n-2\}} + \cdots + p_0^{\min\{n-i,i\}}\right) =$$
$$= (n-1)\, p_0^{\min\{1,n-1\}} + (n-2)\, p_0^{\min\{2,n-2\}} + \cdots + 2\, p_0^{\min\{n-2,2\}} + p_0^{\min\{n-1,1\}}.$$

In the case when $n = 2k$ this sum equals to

$$W_R(C_n) = np_0^{\min\{1,n-1\}} + np_0^{\min\{2,n-2\}} + \cdots + np_0^{\min\{k-1,n-k+1\}} + kp_0^{\min\{k,n-k\}} =$$
$$= np_0^1 + np_0^2 + \cdots + np_0^{k-1} + kp_0^k,$$

and when $n = 2k+1$:

$$W_R(C_n) = np_0^{\min\{1,n-1\}} + np_0^{\min\{2,n-2\}} + \cdots + np_0^{\min\{k-1,n-k+1\}} + np_0^{\min\{k,n-k\}} =$$
$$= np_0^1 + np_0^2 + \cdots + np_0^{k-1} + np_0^k.$$

□

Remark. The case $p_0 = 1$ yields

$$W_R(C_n) = \begin{cases} n(k-1) + k; & n \text{ even}, k = n/2, \\ nk; & n \text{ odd}, k = (n-1)/2 \end{cases} = \binom{n}{2}.$$

Proposition 3 *If* $G = S_n = K_{1,n-1}$ *is a star with* n *vertices* v_1 *(center)*, $v_2, \ldots, v_n$ *and* $p_i = p(v_1, v_{i+1}), i = 1, \ldots, n-1$ *then*

$$W_R(S_n) = \sum_{i=2}^{n} p_{i-1} + \sum_{i=2}^{n}\sum_{j=i+1}^{n} p_{i-1}p_{j-1}.$$

If all link probabilities are equal, $p(e) = p_0$ *for all* $e \in E(G)$, *where* $0 < p_0 \le 1$ *is a constant, then*

$$W_R(S_n) = \binom{n-1}{1} p_0 + \binom{n-1}{2} p_0^2.$$

Proof:

$$\begin{aligned} W_R(S_n) &= \sum_{i=2}^{n} p_0 + \sum_{i=2}^{n}\sum_{j=i+1}^{n} p_0^2 = \\ &= (n-1)p_0 + \sum_{i=2}^{n}(n-i)p_0^2 = \\ &= (n-1)p_0 + \frac{1}{2}(n-1)(n-2)p_0^2 \\ &= \binom{n-1}{1} p_0 + \binom{n-1}{2} p_0^2. \end{aligned}$$

□

Remark. In the case when $p_0 = 1$ we have

$$W_R(S_n) = \binom{n-1}{1} + \binom{n-1}{2} = \binom{n}{2}.$$

Proposition 4 *Define* $G = B_{n,k}$ *as a broom with* n *vertices* $v_1, v_2, \ldots, v_k$ *of a path* P_k *together with* $n-k$ *vertices* $v_{k+1}, v_{k+2} \ldots, v_n$ *all adjacent to the same end vertex* v_k *of a path* P_k. *Let* $p_i = p(v_i, v_{i+1})$ *for* $i = 1, \ldots, k$ *and* $p_i = p(v_k, v_{i+1})$ *for* $i = k+1, \ldots, n-1$. *Then*

$$W_R(B_{n,k}) = W_R(P_k) + W(K_{k,n-k}) + \left(\sum_{i=1}^{k-1} p_i p_{i+1} \cdots p_{k-1}\right) \cdot \left(\sum_{i=k}^{n-1} p_i\right).$$

If all link probabilities are equal, $p(e) = p_0$ *for all* $e \in E(G)$, *where* $0 < p_0 < 1$ *is a constant, then*

$$\begin{aligned} W_R(B_{n,k}) = {} & (k-1)\frac{p_0}{1-p_0} - \left(\frac{p_0}{1-p_0}\right)^2 (1-p_0^{k-1}) + (n-k+1)p_0 + \binom{n-k+1}{2} p_0^2 + \\ & + p_0 \frac{1-p_0^{k-1}}{1-p_0} + (n-k)p_0. \end{aligned}$$

Proof:

$$W_R(B_{n,k}) = W_R(P_k) + W(K_{k,n-k}) + \left(\sum_{i=1}^{k-1} p_0^i\right) \cdot \left(\sum_{i=k}^{n-1} p_0\right) =$$
$$= W_R(P_k) + W(K_{k,n-k}) + p_0 \frac{1-p_0^{k-1}}{1-p_0} + (n-k)p_0.$$

□

Remark. In the case when $p_0 = 1$ we get

$$W_R(B_{n,k}) = W_R(P_k) + W(K_{k,n-k}) + (k-1)(n-k) =$$
$$= \binom{k}{2} + \binom{n-k+1}{2} + (k-1)(n-k) = \binom{n}{2}.$$

Observation 5 *If all link probabilities in connected graph* G *are equal to* 1, $p(e) = 1$ *for all* $e \in E(G)$ *(i.e. all edges are fixed) and* $n = |V(G)|$, *then* $F_{\overrightarrow{uv}} = 1$ *for any* $u, v \in V(G), u \neq v$ *and*

$$W_R(G) = \frac{1}{2}\sum_{u \neq v} F_{\overrightarrow{uv}} = \frac{1}{2}\sum_{u \neq v} 1 = \frac{1}{2} n(n-1) = \binom{n}{2}$$

and this is obviously the upper bound on the reliability Wiener number:

Recall that the Wiener number W is the sum of distances (among all pairs of distinct vertices) and that the minimal value of W is attained for complete graphs, $W(K_n) = \binom{n}{2}$. Hence the upper bound for W_R is at the same time the lower bound for W.

Observation 6 $0 \leq W_R(G) \leq \binom{n}{2} \leq W(G)$.

4. BRANCHING

There is no general agreement about what " *branching*" is and how the extent of branching of the carbon–atoms skeleton of an organic molecule can be represented by some scalar quantity; more details on this matter can be found elsewhere [18, 10, 1, 15]. Anyway, certain conditions that a measure of branching must obey are out of dispute [12, 11].

First, a topological index TI may be acceptable as a measure of branching only if it satisfies the inequalities

$$TI(P_n) > TI(T_n) > TI(S_n) \ , \ n = 5,6,\ldots \tag{2}$$

where P_n and S_n are the n-vertex path graph and star, respectively (see Figure 1), and where T_n is any n-vertex tree, different from P_n and S_n. Indeed, among n-vertex trees P_n is the least branched and S_n the most branched species.

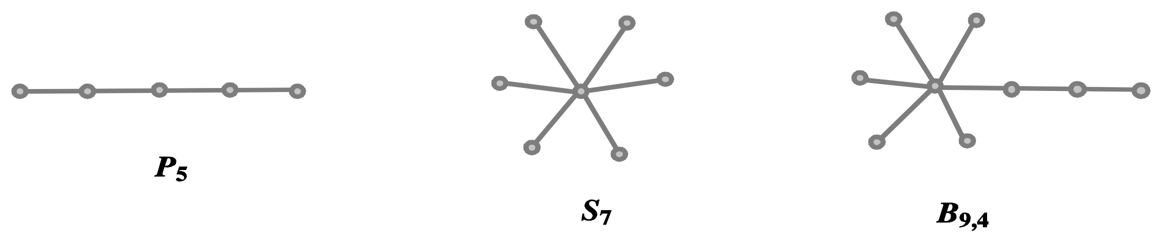

Figure 1: Path P_5, star S_7 and broom $B_{9,4}$.

Second, if T and T^* are graphs whose structure is depicted in Figure 2, then one requires that the inequality

$$TI(T^*) > TI(T) \tag{3}$$

holds irrespective of the actual form of the fragment C . This is because the vertex v_0 in T^* is more branched (has greater degree) than the vertex v_0 in T whereas the other structural details in T and T^* are the same.

Of course, if in Eqs. (2) and (3) all $>$ signs are exchanged by $<$, then the respective TI is equally suitable to measure branching.

In what follows we show that Eqs. (2) and (3) are obeyed by reliability Wiener number.

First, observe that if for $p(e) = 1$ for all edges $e \in E(G)$ then $W_R(P_n) = W_R(S_n)$. Furthermore, if $p(e) = p$ for all edges $e \in E(G)$ then clearly $W_R(P_n) \le W_R(S_n)$. In the sequel, we will consider arbitrary probabilities of edges.

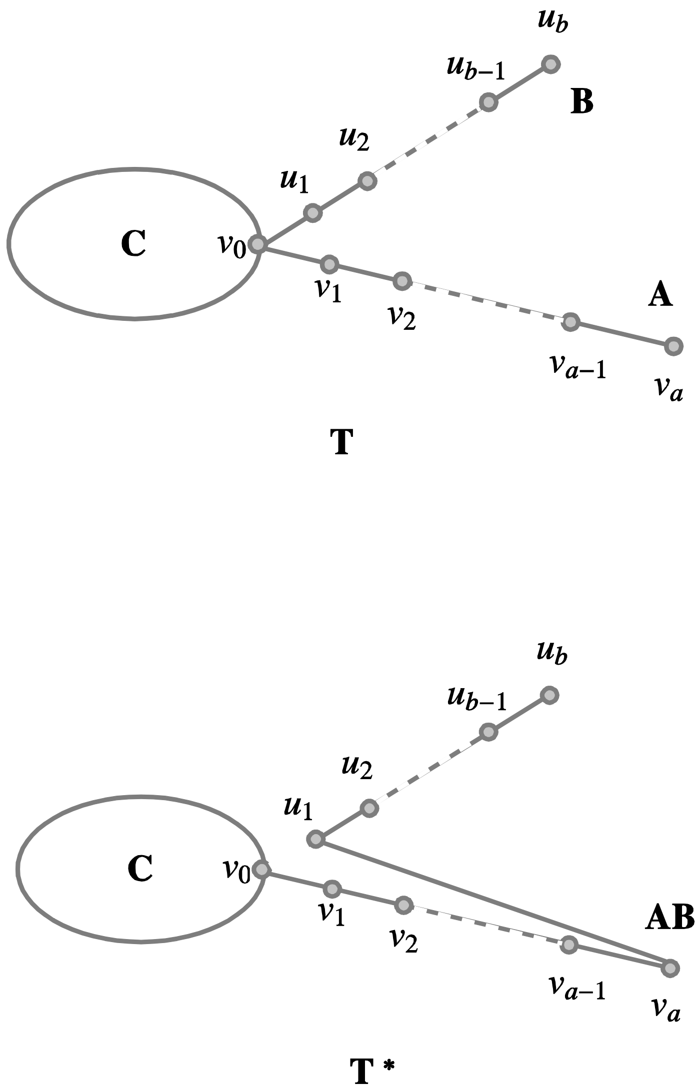

Figure 2: Graphs T and T^*.

Given two disjoint subgraphs F and D of a tree T define

$$W_R(F,D) = \sum_{s\in V(F)} \sum_{r\in V(D)} F_{\overrightarrow{sr}} \tag{4}$$

The following result follows directly from the definition (1):

Lemma 7 *Let T be a tree with subgraphs F and D, $F \cap D = \emptyset$. Denote with F_x a graph F without vertex x and with D_y a graph D without vertex y. Then*

$$W_R(F,D) = W_R(F_x,x)\cdot W_R(x,y)\cdot W_R(y,D_y).$$

In the proof below we will apply the lemma to subgraphs $F, D \in \{\{v_0\}, A, B, \tilde{A}, AB, C\}$.

Recall the labeling of the vertices of the trees T and T^* as indicated in Figure 2. The probabilities of edges are not indicated, and we assume that the probabilities of edges are the same in T and in T^*. In addition, we assume $p(v_a,u_1) = p(v_0,u_1)$.

Theorem 8 *Let the trees T and T^* be defined and labeled as before (see Figure 2). Let A be a path with vertices $\{v_1,v_2,\dots,v_a\}$ and B a path with vertices $\{u_1,u_2,\dots,u_b\}$, both attached to the vertex v_0. Let C denote the rest of the graph, attached to v_0.*
Define the arbitrary weight function p on all edges in T, which remains unchanged in T^*, except $p(v_a,u_1) = p(v_0,u_1)$. Then

$$W_R(T^*) \le W_R(T) \tag{5}$$

provided $W_R(v_a,\tilde{A}) \le W_R(v_0,\tilde{A})$, where $\tilde{A}$ is a path A without vertex v_a.

Proof: We consider the difference $W_R(T) - W_R(T^*)$. From the structure of the trees T and T^* and Lemma 7, we see

$$\begin{aligned}
W_R(T) - W_R(T^*) = \\
&= W_R(v_0,A) + W_R(v_0,B) - W_R(v_0,AB) + \\
&+ W_R(A) + W_R(B) + W_R(A,B) - W_R(AB) + \\
&+ W_R(A,C) + W_R(B,C) - W_R(AB,C) = \\
\\
&= W_R(v_0,B)\cdot[(1 - W_R(v_0,v_a))W_R(v_0,C) + W_R(v_0,\tilde{A}) - W_R(v_a,\tilde{A})] = \\
&= W_R(v_0,B)\cdot[\, W_R(v_0,C) - W_R(v_a,C) + W_R(v_0,\tilde{A}) - W_R(v_a,\tilde{A})\,].
\end{aligned}$$

Using the fact that $W_R(v_0,C) - W_R(v_a,C) \ge 0$ and assuming $W_R(v_0,\tilde{A}) - W_R(v_a,\tilde{A}) \ge 0$, this concludes the proof of Theorem. □

Corollary 9 *In the case when all edge probabilities on A are equal $q = p(v_i,v_{i+1}) = p(v_0,v_1)$ and edge probabilities on B are defined with $p_i = p(u_i,u_{i+1})$, $p_0 = p(v_0,u_1)$ then*

$$W_R(T) - W_R(T^*) = (p_0 + p_0p_1 + \cdots + p_0p_1\cdots p_{b-1})\cdot[(1-q^a)W_R(v_0,C)]$$

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