Fast Computation of the Wiener Index of Fasciagraphs and Rotagraphs

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A matrix approach to the computation of the Wiener index of fasciagraphs and rotagraphs is described. This approach yields efficient algorithms for the above mentioned problem. The running time of our algorithms is independent of the number of monographs, if we regard basic arithmetic operations (such as addition and multiplication) to take a constant time.

1. INTRODUCTION

The notion of a polygraph was introduced in chemical graph theory as a formalization of the chemical notion of polymers.[1] Fasciagraphs and rotagraphs form an important class of polygraphs. In the language of graph theory they describe polymers with open ends and polymers that are closed upon themselves, respectively. They are highly structured, and this structure makes it possible to design efficient algorithms for computing several graph invariants.[2] In this paper we show how the structure of fasciagraphs and rotagraphs can be used to obtain efficient algorithms for computing the Wiener index of such graphs. More precisely, if we regard basic arithmetic operations such as addition and multiplication to take a constant time, then the time complexity of our improved algorithms (theorem 5) depends only on the size k of a monograph in the polygraph and is independent of the number of monographs n.

The paper is organized as follows. Motivation for studying such problems and definitions of polygraphs, rotagraphs, and fasciagraphs are given in section 1. Section 2 describes matrix approach to the computation of the Wiener index of fasciagraphs and rotagraphs. Two basic algorithms that realize this approach are presented (algorithms A and B). In section 3 possible extensions of these algorithms are briefly sketched. Using more sophisticated mathematical methods this approach is further extended, and the two algorithms are considerably improved in section 4. How to realize all these algorithms efficiently is discussed in section 5. The paper ends with some concluding remarks in section 6.

Let $G_1, G_2, ..., G_n$ be arbitrary, mutually disjoint graphs, and let $X_1, X_2, ..., X_n$ be a sequence of sets of unordered pairs of vertices (i.e., edges) such that an edge of X_i joins a vertex of $V(G_i)$ with a vertex of $V(G_{i+1})$. Moreover, we choose edges in X_n to join vertices from $V(G_n)$ with vertices from $V(G_1)$. For convenience we also set $G_{n+1} = G_1$. A *polygraph*

$$\Omega_n = \Omega_n(G_1, G_2, ..., G_n; X_1, X_2, ..., X_n)$$

over *monographs* $G_1, G_2, ..., G_n$ is defined in the following way:

$$V(\Omega_n) = V(G_1) \cup \cdots \cup V(G_n)$$

$$E(\Omega_n) = E(G_1) \cup X_1 \cup E(G_2) \cup X_2 \cup \cdots \cup E(G_n) \cup X_n$$

For a polygraph Ω_n and for $i = 1, 2, ..., n$ we also define

$$L_i = \{u \in V(G_i) \mid \exists v \in V(G_{i+1}) : uv \in X_i\}$$

$$R_i = \{u \in V(G_{i+1}) \mid \exists v \in V(G_i) : uv \in X_i\}$$

In general $R_i \cap L_{i+1}$ need not be empty. In the special case when $G_1, G_2, ..., G_n$ are all isomorphic to a graph G (i.e., all graphs G_i are disjoint copies of the monograph G) and $X_1 = X_2 = ... = X_n = X$ we call the polygraph a *rotagraph* and denote it by $\omega_n(G;X)$. A *fasciagraph* $\phi_n(G;X)$ is defined similarly as a rotagraph $\omega_n(G;X)$ except that there are no edges between the first and the last copy of a monograph, i.e., $X_n = \emptyset$. Since in a rotagraph all the sets L_i and the sets R_i are equal, we will denote them by L and R, respectively. The same notation will be used for fasciagraphs as well, keeping in mind that L_n and R_n are empty.

Throughout the paper we will without loss of generality denote the vertices of a graph G by 1, 2, ..., k. Recall that the Wiener index is defined for an arbitrary connected graph G as follows. Let $D(G) = [d_{ij}]$ be the distance matrix of G,

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i.e., the $k \times k$ matrix whose entry d_{ij} is equal to the length of a shortest path in G between vertices i and j. The Wiener index $W(G)$ of G is the number

$$W(G) = \sum_{i=1}^{k} \sum_{j=i+1}^{k} d_{ij} = \frac{1}{2}\sum_{i=1}^{k} \sum_{j=1}^{k} d_{ij}$$

This index was introduced in 1947.[3] Although it was the first topological index studied, even today it is a very widely employed graph theoretical descriptor.[4] In addition to conventional applications, the recent studies show its applicability in the prediction of ultrasonic sound velocities in alkanes and alcohols,[5] the rate of electroreduction of chlorobenzenes,[6] cytostatic and antihistaminic activities of certain drugs,[7] and the discrimination of various fullerene isomers.[8] The Wiener index of polymer molecular graphs that correspond to our notion of polygraphs has been studied in refs 9−11. Regarding the computation of the Wiener index see, e.g., refs 12−16.

2. THE BASIC ALGORITHM

The theory of path algebras[17] was used in ref 2 to derive a general algorithm for computing some graph invariants on polygraphs including the domination number and the independence number and solving the k-colorability decision problem. The general idea of the algorithm of Klavžar and Žerovnik is to transform the problem of computing a particular graph invariant on a polygraph to the computation of certain matrix products, where the matrix product is defined in a nonstandard way depending on the particular problem to be solved. The present paper applies the same idea to the problem of computing the Wiener index. In this paper, however, we try to avoid the general theory and give only the definitions which are necessary to make the following presentation self-contained.

We wish to remark that similar ideas were already used by some authors. Babić, Graovac, Mohar, and Pisanski give formulas for the matching polynomial of a polygraph involving the trace of a certain matrix product,[1] and Gutman, Kolaković, Graovac and Babić present a method for computing the Hosoya index of polymers.[18] Our method is also similar to the transfer matrix methods as described, e.g., in ref 19.

We consider matrices with entries from the set $\mathbb{N}_0 \cup \{\infty\}$, i.e., we add to the set of nonnegative integers a special element ∞ called infinity. For an $n \times p$ matrix A and an $p \times m$ matrix B we define their product $C = A \circ B$ of size $n \times m$ as

$$(C)_{ij} = \min_{1 \le s \le p} ((A)_{is} + (B)_{sj}) \tag{1}$$

For an extensive survey of (mathematical) results and a thorough development of the theory concerning the above matrix product the interested reader is invited to consult ref 20.

Let $\psi_n(G;X)$ and $\omega_n(G;X)$ be a fasciagraph and a rotagraph, respectively, and recall that $V(G) = \{1, 2, .., k\}$. Define a $k \times k$ transition matrix $A(X) = [a_{ij}]$ in the following way:

$$a_{ij} = \begin{cases} 1; & i \in L, j \in R, \text{and } ij \in X \\ \infty; & \text{otherwise} \end{cases}$$

Note that $i \in L$ belongs to some monograph G, while $j \in R$ belongs to the next copy of G.

The Wiener index of $\phi_n(G;X)$ can be computed by the following algorithm:

Algorithm A

1. compute $D_0 := D(G)$
2. determine $A(X)$
3. for $l = 1, 2, ..., n - 1$ do $D_l := D_{l-1} \circ A(X) \circ D_0$
4. $s_0 := \sum_{i=1}^{k} \sum_{j=i+1}^{k} d_{ij}$
5. for $l = 1, 2, ..., n - 1$ do $s_l := \sum_{i=1}^{k} \sum_{j=1}^{k} (D_l)_{ij}$
6. $W(\psi_n(G;X)) := \sum_{i=0}^{n-1} (n - i)s_i$

To prove the correctness of the above algorithm we need an additional assumption that each copy of a monograph G is an isometric subgraph of $\psi_n(G;X)$. A subgraph H of a graph G is an *isometric* subgraph, if the distance between any two vertices of H in G is achieved by a shortest path which lies completely in the subgraph H. Isometric subgraphs and isometric embeddings of graphs form an important part of graph theory. We refer to ref 21 for a survey on results and applications of isometric subgraphs.

Theorem 1. *Suppose that each copy of the monograph G is a connected isometric subgraph of the fasciagraph $\psi_n(G;X)$. Then algorithm A correctly computes the Wiener index of $\psi_n(G;X)$.*

Proof. Consider the fasciagraph $\psi_n(G;X)$. Observe first that because of the obvious symmetry and since each monograph is an isometric subgraph, the distance between any two vertices from G_i and G_j, $i < j$, and the corresponding two vertices from $G_{i'}$ and $G_{j'}$, $i' < j'$, coincide if $j - i = j' - i'$. Therefore it is enough to compute the distances between the first and any other copy of the monograph.

We claim that matrices D_l, $l = 0, 1, ..., n - 1$, calculated in steps 1 and 3 of the algorithm contain distances in $\psi_n(G;X)$ between all pairs of vertices i, j, where $i \in V(G_1)$ and $j \in V(G_{l+1})$. The claim is true for $l = 0$ by the definition of D_0 and the isometry assumption. Suppose now that the claim holds for $l - 1$, $l \ge 1$ and consider the equality $D_l = D_{l-1} \circ A(X) \circ D_0$. Then

$$(D_l)_{ij} = \min_{1 \le s \le k} ((D_{l-1})_{is} + (A(X) \circ D_0)_{sj})$$

By the induction hypothesis, $(D_{l-1})_{is}$ is the length of a shortest path between vertices i and s, where $i \in V(G_1)$ and $s \in V(G_l)$. Observe finally that $(A(X) \circ D_0)_{sj}$ is the length of a shortest path that does not use any edge of G_l between s (considered as a vertex in $V(G_l)$) and the vertex $j \in V(G_{l+1})$. This implies the claim.

It follows from the claim that the distance matrix of the fasciagraph $\psi_n(G;X)$ can be written in the block form

$$\begin{bmatrix} D_0 & D_1 & D_2 & \cdots & D_{n-1} \\ D_1^T & D_0 & D_1 & \cdots & D_{n-2} \\ D_2^T & D_1^T & D_0 & \cdots & D_{n-3} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ D_{n-1}^T & D_{n-2}^T & D_{n-3}^T & \cdots & D_0 \end{bmatrix}$$

where D_l^T is the transpose of the matrix D_l. Now it is clear that step 6 correctly computes $W(\psi_n(G;X))$.

Note that it also follows from the above proof that

$$D_{i+j} = D_i \circ D_j, \quad i, j \geq 0$$

To compute the Wiener index of $\omega_n(G;X)$ we will use the same idea as in algorithm A. However, we have to take care of some additional details. Let u and v be vertices from different copies of G. Then we must consider two possible directions to connect u and v by a shortest path. If $u \in V(G_i)$ and $v \in V(G_j)$, $i < j$, then a shortest path between u and v can pass through monographs $G_i, G_{i+1}, ..., G_{j-1}, G_j$ (the first direction) or through monographs $G_i, G_{i-1}, ..., G_1, G_n, ..., G_{j+1}, G_j$ (the second direction). In the presentation we will use the same notation as in algorithm A, except that instead of D_l we will have two distance matrices D_l and D_l', where D_l' will contain the distances between the vertices of G_1 and G_{l+1} in the first direction and D_l will contain the distances between the same pairs of vertices in the whole rotagraph $\omega_n(G;X)$. Observe that the distances in the second direction are closely related to the distances in the first direction since $D_l'^T$ is the distance matrix between the vertices of G_{l+1} and G_1 in the second direction. This way algorithm A extends to the case of rotagraphs as follows.

Algorithm B

1. compute $D_0 = D_0' := D(G)$

2. determine $A(X)$

3. for $l = 1, 2, ..., n-1$ do $D_l' := D_{l-1}' \circ A(X) \circ D_0$

4. for $l = 1, 2, ..., n-1$ do $D_l := \min\{D_l', D_{n-l}'^T\}$,
where $(\min\{A,B\})_{ij} = \min\{(A)_{ij},(B)_{ij}\}$

5. $s_0 := \sum_{i=1}^{k} \sum_{j=i+1}^{k} d_{ij}$

6. for $l = 1, 2, ..., n-1$ do $s_l := \sum_{i=1}^{k}\sum_{j=1}^{k}(D_l)_{ij}$

7. $W(\omega_n(G;X)) := n s_0 + \frac{n}{2}\sum_{i=1}^{n-1} s_i$

To show the correctness of the above algorithm we need the same assumption on the monographs as in theorem 1.

Theorem 2. *Suppose that each copy of the monograph G is a connected isometric subgraph of the rotagraph $\omega_n(G;X)$. Then algorithm B correctly computes the Wiener index of $\omega_n(G;X)$.*

The proof of the theorem is very similar to the case of fasciagraphs, and we will therefore omit the details. We note, however, that step 7 is simplified compared to step 6 of algorithm A because of the circular symmetry of rotagraphs.

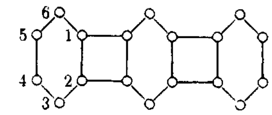

Figure 1. The fasciagraph H_3.

In fact, algorithm B can be made more efficient by observing the following facts. First note that if $s \geq t$, then

$$(D_s')_{ij} - (D_t')_{ij} \geq s - t$$

Hence, for $l \leq n/2$ we have

$$(D_l')_{ij} \leq (D_{n-l}')_{ij} + 2l - n = (D_{n-l}'^T)_{ji} + 2l - n$$

Since $(D_{n-l}'^T)_{ji}$ is at most $(D_{n-l}'^T)_{ij}$ plus twice the diameter of the monograph G, which is in turn bounded by $k - 1$, we conclude that

$$(D_l')_{ij} \leq (D_{n-l}'^T)_{ij} + 2(k-1) + 2l - n$$

The above inequality implies that $\min\{D_l', D_{n-l}'^T\} = D_l'$ for $l \leq [n/2] - k + 1$. Analogously, $\min\{D_l', D_{n-l}'^T\} = D_{n-l}'^T$ for $l \geq [(n+1)/2] + k - 1$. Therefore to determine the matrices $D_0, ..., D_{n-1}$ it is enough to compute the matrices D_l' only up to $l = [(n-3)/2] + k$.

Example 1. Consider the fasciagraph H_3 shown in Figure 1 where the vertices of the first copy of the monograph C_6 are labeled as indicated. Note that the monographs are isometric subgraphs of H_3.

The matrices $D_0 = D(G)$ and $A(X)$ are

$$\begin{bmatrix} 0 & 1 & 2 & 3 & 2 & 1 \\ 1 & 0 & 1 & 2 & 3 & 2 \\ 2 & 1 & 0 & 1 & 2 & 3 \\ 3 & 2 & 1 & 0 & 1 & 2 \\ 2 & 3 & 2 & 1 & 0 & 1 \\ 1 & 2 & 3 & 2 & 1 & 0 \end{bmatrix} \text{ and } \begin{bmatrix} \infty & \infty & \infty & \infty & 1 & \infty \\ \infty & \infty & \infty & 1 & \infty & \infty \\ \infty & \infty & \infty & \infty & \infty & \infty \\ \infty & \infty & \infty & \infty & \infty & \infty \\ \infty & \infty & \infty & \infty & \infty & \infty \\ \infty & \infty & \infty & \infty & \infty & \infty \end{bmatrix}$$

while the matrices D_1 and D_2 are equal to

$$\begin{bmatrix} 3 & 4 & 3 & 2 & 1 & 2 \\ 4 & 3 & 2 & 1 & 2 & 3 \\ 5 & 4 & 3 & 2 & 3 & 4 \\ 6 & 5 & 4 & 3 & 4 & 5 \\ 5 & 6 & 5 & 4 & 3 & 4 \\ 4 & 5 & 4 & 3 & 2 & 3 \end{bmatrix} \text{ and } \begin{bmatrix} 6 & 7 & 6 & 5 & 4 & 5 \\ 7 & 6 & 5 & 4 & 5 & 6 \\ 8 & 7 & 6 & 5 & 6 & 7 \\ 9 & 8 & 7 & 6 & 7 & 8 \\ 8 & 9 & 8 & 7 & 6 & 7 \\ 7 & 8 & 7 & 6 & 5 & 6 \end{bmatrix}$$

Then $s_0 = 27$, $s_1 = 126$, $s_2 = 234$, and $W(H_3) = 3s_0 + 2s_1 + s_2 = 567$.

Consider next the rotagraph H_3' which we get from H_3 by adding two additional edges between the last and the first monograph. Since in our example both directions are equivalent, we have $D_l' = D_l'^T$ and consequently $s_1 = s_2$. Then $W(H_3') = 3s_0 + {}^3/_2(s_1 + s_2) = 3s_0 + 3s_1 = 459$.

3. NONISOMETRIC MONOGRAPHS

It is possible to extend algorithms A and B also to the case when monographs are not isometric subgraphs of the polygraph. However, we still need a much weaker assumption, namely that the polygraph is "locally connected", which means that any pair of vertices in the same monograph is at distance at most d for some constant d independent of n. In such a case a shortest path between two vertices $u, v \in V(G_i)$ can leave G_i. But since the distance between u and v is at most d, such a path can use only monographs $G_{i-[d/2]}, ..., G_{i+[d/2]}$. This implies that the distance matrices of the monographs G_i, $[d/2] < i \le n - [d/2]$, in the fasciagraph and all distance matrices of the monographs in the rotagraph are identical. Moreover, they can be computed efficiently by considering only a small portion of the polygraph, namely, only at most $d + 1$ successive monographs.

Following the above discussion, algorithm B remains unchanged except that in step 1 the matrix D_0 $(= D_0')$ has to be computed as described above, i.e., $(D_0)_{ij}$ must be the distance in $\omega_n(G;X)$ between the vertices i and j from G_0.

When considering fasciagraphs with nonisometric monographs, we have to perform some additional changes. Since fasciagraphs do not possess the circular symmetry of rotagraphs, the first and the last $[k/2]$ copies of monographs have to be considered separately. Because of these exceptional monographs the generalization of algorithm A is more complicated and less practical.

4. FURTHER IMPROVEMENTS

Using more sophisticated mathematical reasoning it is possible to further improve the above procedures for determining the Wiener index of fasciagraphs and rotagraphs.

Consider a fasciagraph $\psi_n(G;X)$ and let $\mathscr{D} = \{D_0, ..., D_{n-1}\}$ be the set of distance matrices determined by algorithm A. We would like to show that for large enough indices l matrices D_l have a special structure that enables us to compute the Wiener index efficiently. For this purpose, let us define a relation $\sim$ on $\mathscr{D}$ by the requirement $A \sim B$ if and only if $A - B$ is a constant matrix, i.e., a matrix with all entries equal. It is easy to check that $\sim$ is an equivalence relation on $\mathscr{D}$. Moreover, the chosen matrix product $\circ$ is compatible with $\sim$ in the following sense.

Lemma 3. *Let A, B, and C be matrices of size $k \times k$ with C being a constant matrix. Then*

$$(A + C) \circ B = A \circ B + C$$

Proof. Denote by c the entries of the constant matrix C. By the definition of $\circ$ we have

$$\begin{aligned} ((A + C) \circ B)_{ij} &= \min_{1 \le l \le k} ((A + C)_{il} + (B)_{lj}) \\ &= \min_{1 \le l \le k} ((A)_{il} + c + (B)_{lj}) \\ &= \min_{1 \le l \le k} ((A)_{il} + (B)_{lj}) + c = (A \circ B)_{ij} + c \end{aligned}$$

which proves the claim.

The number of equivalence classes that $\mathscr{D}$ is partitioned into by $\sim$ is bounded by $(2k - 1)^{k^2}$. This is easily proved by using the fact that the difference between any two elements of an arbitrary matrix D_l cannot be greater than $2k - 2$. The number of distinct equivalence classes is thus bounded by a (possibly large) constant that depends only on the size k of a single monograph and is independent of the number n of monographs. Therefore if n is large enough, there is the first index q such that the matrix D_q is equivalent to some previous matrix, say D_p. Note that $q \le (2k - 1)^{k^2}$ is bounded independently of n. Denote by C the constant matrix $C = D_q - D_p$ and set $P = q - p$.

Lemma 4. *Let p, P, and C be defined as above. Then for every $i \ge p$ and every $j \ge 0$ such that $i + jP \le n$ we have*

$$D_{i+jP} = D_i + jC$$

Proof. We will prove the claim by double induction on j and i. If $j = 0$, there is nothing to prove. Consider now the case $j = 1$. If $i = p$, then the claim holds by the definition of P. Suppose now that $D_{i-1+P} = D_{i-1} + C$. Then

$$\begin{aligned} D_{i+P} &= D_{i-1+P} \circ (A(X) \circ D_0) \\ &= (D_{i-1} + C) \circ (A(X) \circ D_0) \\ &= D_{i-1} \circ (A(X) \circ D_0) + C = D_i + C \end{aligned} \qquad (2)$$

Note that induction hypothesis was used at the second equality and that lemma 3 with $A = D_{i-1}$ and $B = A(X) \circ D_0$ was applied at the third one. Therefore the claim is true also for $j = 1$.

Suppose that the assertion holds for $j - 1$, $D_{i+(j-1)P} = D_i + (j - 1)C$. Then again by induction hypothesis and by (2) where we use $i + (j - 1)P$ in the place of i we have

$$D_{i+jP} = D_{i+(j-1)P+P} = D_{i+(j-1)P} + C = D_i + (j - 1)C + C = D_i + jC$$

Now we are ready to state our main result, an explicit formula for the Wiener index of fasciagraphs.

Theorem 5. *Let G be a connected graph with k vertices and suppose that each copy of G is an isometric subgraph of $\psi_n(G;X)$. Define p, q, P, and C as above and let all entries of C be equal to c. Set $m = [(n - p)/P]$ and let $r = n - 1 - mP$. Then*

$$W(\psi_n(G;X)) = \sum_{i=0}^{r} (n - i)s_i + m\sum_{i=1}^{P}\left(n - r - \frac{(m - 1)P}{2} - i\right)s_{r+i} + \frac{k^2 c(m - 1)mP}{2}\left(n - r - \frac{(2m - 1)P}{3} - \frac{P + 1}{2}\right)$$

Proof. Observe first that our definitions of m and r imply $p - 1 \le r < q - 1$. Following algorithm A, the Wiener index $W = W(\psi_n(G;X))$ can be expressed as $W = W_1 + W_2$, where

$$W_1 = \sum_{i=0}^{r} (n - i)s_i \quad \text{and} \quad W_2 = \sum_{i=r+1}^{n-1} (n - i)s_i$$

Using lemma 4 the term W_2 can be further transformed into

$$\begin{aligned} W_2 &= \sum_{i=r+1}^{n-1} (n - i)s_i = \sum_{i=0}^{m-1}\sum_{j=1}^{P} (n - r - iP - j)s_{r+iP+j} \\ &= \sum_{i=0}^{m-1}\sum_{j=1}^{P} (n - r - iP - j)(s_{r+j} + ik^2c) \end{aligned}$$

Now a routine calculation shows that

$$W_2 = m\sum_{j=1}^{P}\left(n - r - \frac{(m-1)P}{2} - j\right)s_{r+j} + \frac{k^2c(m-1)mP}{2}\left(n - r - \frac{(2m-1)P}{3} - \frac{P+1}{2}\right)$$

which we have claimed.

Theorem 5 implies that in order to obtain the Wiener index of a given fasciagraph it is enough to compute only the matrices D_0, ..., D_{r+P}, where P and r are defined as previously. Let us recall that r and P cannot be too large, i.e., there is an upper bound on r and P that is independent of the number of monographs n. For n large enough this considerably improves algorithm A, which requires all matrices D_0, ..., D_{n-1} to be computed.

The results of theorem 5 can also be extended to the case when monographs are connected but not isometric subgraphs of the fasciagraph. As mentioned in section 3, in such a case the first and the last $[k/2]$ monographs have to be considered separately, and this additional requirement increases the complexity of the obtained formula.

Let us illustrate the use of theorem 5 by an example.

Example 2. Consider a fasciagraph H_n obtained by taking n monographs C_6 connected as in Figure 1 for the case $n = 3$. From calculations in example 1 it follows that $D_2 = D_1 + C$ where C is a constant matrix with all entries equal to 3. Therefore we have $k = 6$, $p = 1$, $q = 2$, $P = 1$, $c = 3$, $m = n - 1$, and $r = 0$. Applying theorem 5 we get

$$\begin{aligned} W(H_n) &= ns_0 + \frac{1}{2}(n-1)ns_1 + 18(n-2)(n-1)n \\ &= n(27 + 63(n-1) + 18(n-2)(n-1)) \\ &= 9n^2(2n+1) \end{aligned}$$

As expected, for $n = 3$ this gives $W(H_3) = 567$.

The same ideas can also be applied in the case of rotagraphs. Let s_l' be defined by the formula in step 6 of algorithm B where D_l' is taken instead of D_l. Following algorithm B and the discussion after it, the Wiener index $W = W(\omega_n(G;X))$ of a rotagraph $\omega_n(G;X)$ can be expressed as $W = n(2W_1 + W_2)/2$, where

$$W_1 = \sum_{i=0}^{N} s_i', \quad W_2 = \sum_{i=N+1}^{n-N-1} s_i$$

and $N = [n/2] - k + 1$. Here we have used the fact that the sum of elements of $D_l'^{\mathrm{T}}$ is the same as in D_l'. The first term can be handled similarly as the whole Wiener index in theorem 5. If we take $n' = N + 1$ and adopt the meaning of p', q', P', c', m' and r' from theorem 5 with respect to the sequence of matrices D_0', D_1', ..., $D_{n'-1}'$, we have

$$\begin{aligned} W_1 &= \sum_{i=0}^{r'} s_i' + \sum_{i=r'+1}^{n'-1} s_i' = \sum_{i=0}^{r'} s_i' + \sum_{i=0}^{m'-1}\sum_{j=1}^{P'} s_{r'+iP'+j}' \\ &= \sum_{i=0}^{r'} s_i' + \sum_{i=0}^{m'-1}\sum_{j=1}^{P'} (s_{r'+j}' + ik^2c') \\ &= \sum_{i=0}^{r'} s_i' + m'\sum_{i=1}^{P'} s_{r'+i}' + P'k^2c'\frac{(m'-1)m'}{2} \end{aligned}$$

Note that parameters p', q', P', c', m', and r' are the same for both sequences of matrices D_0', ..., $D_{n'-1}'$ and $D_0'^{\mathrm{T}}$, ..., $D_{n'-1}'^{\mathrm{T}}$.

The sum W_2 contains at most $2k - 2$ terms. Since D_{N+1}' (and hence also s_{N+1}) can be computed with a small number of arithmetic operations using the above techniques, W_2 can also be computed efficiently.

Let us illustrate the above discussion by an example.

Example 3. Consider the rotagraph H_n' obtained from the fasciagraph H_n of example 2 by adding two edges between the last and the first copy of the monograph C_6. Since both directions in H_n' are equivalent, we have $D_l' = D_l'^{\mathrm{T}}$. From the calculations in previous examples we already know that $D_2' - D_1' = C$ is the constant matrix with all entries equal to 3. Hence for every $l \geq 1$ we have $(D_{l+1}')_{ij} > (D_l')_{ij}$. Let us remark that this property is not true for arbitrary fasciagraphs or rotagraphs even if each monograph is an isometric subgraph. We leave it to the interested reader to construct such an example. On the other hand, it is always true that $(D_{l+P'}')_{ij} > (D_l')_{ij}$. Now it follows that $D_l = D_l'$ for $l \leq [n/2]$ and $D_l = D_{n-l}'^{\mathrm{T}}$ for $l > [n/2]$. This enables us to take $n' = [(n-1)/2] + 1$ and henceforth reduce the term W_2 to 0 if n is odd, and to $s_{n/2}$ if n is even. Since $k = 6$, $p' = 1$, $q' = 2$, $P' = 1$, $c' = 3$, $r' = 0$, and $m' = n' - 1$, we have $W_1 = 9(6n'^2 - 4n' + 1)$ and also $s_{n/2} = 18 + 54n$ when n is even. Summing up these two expressions (when necessary) and multiplying the sum by $n/2$ we get

$$W(H_n') = 9n\left(3\left[\frac{n^2}{2}\right] + n + 2\right)$$

As expected, for $n = 3$ this gives $W(H_3') = 459$.

5. COMPUTING THE MATRICES D_l FASTER

If only a particular distance matrix, say D_l, is needed, it is possible to further optimize the complexity of computation. Recall that $D_l = D_{l-1} \circ A(X) \circ D_0$, $l \geq 1$, and hence

$$D_l = D_0 \circ (A(X) \circ D_0)^l$$

It is well-known (ref 22, p 399) that for fast computation of the lth power of a matrix at most $2\log_2 l$ matrix products have to be computed. The complexity of computing a matrix product depends on the size of the matrices involved. In our case, the dimension of $A(X) \circ D_0$ is equal to the number of vertices of G. We show in this section that it is possible to compute D_l by computing the power of a smaller matrix of size which equals the number of vertices in L (or in R, if this set is smaller). If the number of vertices in L (or in R) is much smaller than the number of vertices of the monograph G, this gives a considerable saving in the computation time.

In example 1 many elements of the matrix $A(X)$ are equal to the special element ∞. This causes a lot of redundant computation that can be avoided. The rows in $A(X) \circ D_0$ corresponding to the vertices not involved as endpoints of edges given by X are trivial, i.e., have all elements equal to ∞. Analyzing the computation which is really needed in example 1 we see that we need to compute only powers of a matrix of size 2×2 and not of size 6×6.

The general idea uses the above observation. Let us call a row (column) of $A(X)$ with all elements equal to ∞ *trivial*.

Label the nontrivial rows and columns with $i_1, i_2, ..., i_t$ and $j_1, j_2, ..., j_{t'}$, respectively.

$$A(X) = \begin{array}{c} \left[\begin{array}{cccccc} & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \end{array} \right] \\ \uparrow \; \uparrow \; \uparrow \; \uparrow \; \uparrow \; \uparrow \\ \underbrace{j_1 \; j_2 \; \cdots \; j_{t'}}_{\text{columns with at least one 1}} \end{array} \begin{array}{l} \leftarrow i_1 \\ \leftarrow i_2 \\ \leftarrow \\ \leftarrow \vdots \\ \leftarrow \\ \leftarrow i_t \end{array} \left.\vphantom{\begin{array}{l} a \\ a \\ a \\ a \\ a \\ a \end{array}}\right\} \text{rows with at least one 1}$$

Let

$$\hat{A} = \widehat{A(X)}$$

be the matrix obtained from $A(X)$ by deleting all trivial rows and columns. Hence $\hat{A}$ is of size $t \times t'$. Then

$$A(X) = M \circ \hat{A} \circ M'$$

where M is of size $k \times t$ and is obtained from the matrix

$$I = \begin{bmatrix} 0 & \infty & \infty & \cdots & \infty \\ \infty & 0 & \infty & \cdots & \infty \\ \infty & \infty & 0 & \cdots & \infty \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \infty & \infty & \infty & \cdots & 0 \end{bmatrix}$$

of size $k \times k$ by taking the columns $i_1, i_2, ..., i_t$ and M' is of size $t' \times k$ and is obtained from I by taking the rows $j_1, j_2, ..., j_{t'}$.

For the matrix $A(X)$ from example 1 we have $A(X) = M \circ \hat{A} \circ M'$, where

$$M = \begin{bmatrix} 0 & \infty \\ \infty & 0 \\ \infty & \infty \\ \infty & \infty \\ \infty & \infty \\ \infty & \infty \end{bmatrix}, \hat{A} = \begin{bmatrix} \infty & 1 \\ 1 & \infty \end{bmatrix}, M' = \begin{bmatrix} \infty & \infty & \infty & 0 & \infty & \infty \\ \infty & \infty & \infty & \infty & 0 & \infty \end{bmatrix}$$

Example 4. The matrix

$$A(X) = \begin{bmatrix} \infty & 1 & \infty & 1 & \infty \\ \infty & 1 & \infty & \infty & \infty \\ \infty & \infty & 1 & \infty & 1 \\ \infty & \infty & 1 & \infty & \infty \\ \infty & \infty & \infty & \infty & \infty \end{bmatrix}$$

can be written as $A(X) = M \circ \hat{A} \circ M'$, where

$$\hat{A} = \begin{bmatrix} 1 & \infty & 1 & \infty \\ 1 & \infty & \infty & \infty \\ \infty & 1 & \infty & 1 \\ \infty & 1 & \infty & \infty \end{bmatrix}, \quad M = \begin{bmatrix} 0 & \infty & \infty & \infty \\ \infty & 0 & \infty & \infty \\ \infty & \infty & 0 & \infty \\ \infty & \infty & \infty & \infty \end{bmatrix},$$

$$M' = \begin{bmatrix} \infty & 0 & \infty & \infty & \infty \\ \infty & \infty & 0 & \infty & \infty \\ \infty & \infty & \infty & 0 & \infty \\ \infty & \infty & \infty & \infty & 0 \end{bmatrix}$$

The matrices D_l can thus be expressed in terms of $D = D_0$, M, M', and $\hat{A}$ as follows:

$$D_1 = D \circ A \circ D = D \circ M \circ \hat{A} \circ M' \circ D$$

$$\begin{aligned} D_2 &= D_1 \circ A \circ D \\ &= D \circ M \circ \hat{A} \circ (M' \circ D \circ M) \circ \hat{A} \circ M' \circ D \\ &= D \circ M \circ \hat{A} \circ \hat{D} \circ \hat{A} \circ M' \circ D \end{aligned}$$

where $\hat{D} = M' \circ D \circ M$. By induction we have

$$\begin{aligned} D_l &= D_{l-1} \circ A \circ D \\ &= D \circ M \circ (\hat{A} \circ \hat{D})^{l-2} \circ (\hat{A} \circ M' \circ D \circ M) \circ \hat{A} \circ M' \circ D \\ &= D \circ M \circ (\hat{A} \circ \hat{D})^{l-1} \circ \hat{A} \circ M' \circ D \end{aligned} \quad (3)$$

The size of the matrix $\hat{D}$ is $t' \times t$ and hence the size of the matrix $\hat{A} \circ \hat{D}$ is $t \times t$. Similarly,

$$D_l = D \circ M \circ \hat{A} \circ (\hat{D} \circ \hat{A})^{l-1} \circ M' \circ D$$

Now the size of the matrix $\hat{D} \circ \hat{A}$ is $t' \times t'$.

Therefore, to compute any D_l, the $(l - 1)$th power of a "small" matrix of size $t \times t$ (or $t' \times t'$) is needed in addition to a constant number (five) of "larger" matrix products.

6. CONCLUSIONS

It is possible to extend the results of this paper also to the case when monographs are not isometric subgraphs of the polygraph (see section 3). But since such extended algorithms would be much more involved than the presented ones, it seems that such a generalization is short of practical value.

Distances between a fixed vertex and all other vertices of a graph are usually computed using a breadth-first search.[12,23] Our algorithms A and B (with improvements presented in section 5) are roughly of the same time complexity with the difference that they are formulated in the language of matrices instead of in the language of graph theory. As an additional advantage, this matrix approach enables us to further improve the designed algorithms in a very simple way.

The problem treated in this paper is a particular case of the so-called path problems.[17] The path problems are frequently encountered in operations research and the examples are given by problems of the shortest path, the longest path, the path with the maximum capacity, the listing of all possible paths, etc. For each particular problem a suitable abstract algebraic structure is introduced. Here it has been shown that by using the binary operation defined by the equation (1), one can develop an algorithm that computes the Wiener index of rotagraphs and fasciagraphs efficiently.

Before closing we would like to point out that it is possible to use this approach for computing the Wiener index of arbitrary polygraphs, too. In this case, each monograph G_i, $1 \le i \le n$, of a polygraph $\Omega_n = \Omega_n(G_1, G_2, ..., G_n; X_1, X_2, ..., X_n)$ has its own distance matrix $D_0^{(i)}$ and each edge set X_i is associated with its transition matrix $A^{(i)} = A(X_i) = [a_{uv}^{(i)}]$, where

$$a_{uv}^{(i)} = \begin{cases} 1; & u \in L_i, v \in R_i \text{ and } uv \in X_i \\ \infty; & \text{otherwise} \end{cases}$$

Similarly as in algorithm B, denote by $D_l'^{(i)}$ the matrix containing distances between vertices of the monographs G_i

and G_{i+l} in the first direction. Then $D'^{(i)}_0 = D^{(i)}_0$ and

$$D'^{(i)}_l = D'^{(i)}_0 \circ A^{(i)} \circ D'^{(i+1)}_{l-1} = D'^{(i)}_{l-1} \circ A^{(i+l-1)} \circ D'^{(i+l)}_0$$

As before, the distances in the second direction are easily obtained using the distance matrices $D'^{(i)}_l$. Finally, for every i, $1 \le i \le n$

$$D^{(i)}_l = \min\{D'^{(i)}_l, D'^{(i+l)\mathrm{T}}_{n-l}\}$$

is the required matrix containing distances between vertices of the monographs G_i and G_{i+l} in the polygraph Ω_n.

This approach yields an algorithm of time complexity $O(n^2)$ which is no better than the well-known general methods for arbitrary graphs.[12] However, if a polygraph does not have many nonisomorphic monographs, then it still may be possible to gain some savings in computation time from the approach applied in this paper. Moreover, this approach seems to be quite suitable for parallel computations.

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