Distance-related invariants on polygraphs

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Abstract

Let $M^{(n)}$ be a graph which is obtained from a path P_n or a cycle C_n by replacing each vertex by a fixed graph M and replacing each edge by a fixed set of edges joining the corresponding copies of M. A matrix approach to the computation of distance related invariants in such graphs is presented. This approach gives a general procedure to obtain closed formulas (depending on n) for such invariants of $M^{(n)}$. As an example, the Wiener index is treated in more details.

1 Introduction

The notion of a polygraph was introduced in chemical graph theory as a formalization of the chemical notion of polymers [2]. Fasciagraphs and rotagraphs form an important class of polygraphs. They describe polymers with open ends and polymers that are closed upon themselves, respectively. Their special structure makes it possible to design

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efficient procedures for computing several graph invariants [10]. It was shown in [9] how the structure of fasciagraphs and rotagraphs can be used to obtain efficient algorithms for computing the Wiener index of such graphs (under some additional constraints).

In this paper we use the same approach to study a general class of distance related graph invariants. We initiate development of a general theory of such invariants on infinite chain graphs. The results are illustrated on a well-known distance-related graph invariant, the Wiener index, for which general formulas for rotagraphs and fasciagraphs are derived. Similar approach can be used also for other distance-related graph invariants.

The structure of the paper is as follows. In Section 2 we study infinite chain graphs which can be viewed as host graphs or coverings of fascia and rotagraphs, respectively. The main result of Section 2 is Theorem 2.3 which shows that the connectivity of the infinite chain graph is a "local property". The derived bound on "locality" is shown to be best possible. In Section 3 we relate fascia and rotagraphs to the infinite chain graphs, and in Sections 4 and 5 we conclude by showing how one obtains closed formulas for the Wiener index (and more general distance-related graph invariants) of polygraphs.

2 Distances in infinite chain graphs

In this section we introduce infinite chain graphs and prove some general results on connectivity and (partial) distance matrices in such graphs (Proposition 2.2, Theorem 2.3, and Proposition 2.4). The key observation is Proposition 2.4 which is the main ingredient of efficient computational procedures presented in later sections.

Let M be a fixed graph (also called *monograph*) with k vertices and let $X \subseteq V(M) \times V(M)$ be a nonempty binary relation on the vertices of M. Denote by $\mathbf{Z}$ the set of integers. The *infinite chain graph* $\Xi = \Xi(M, X)$ based on M and X is defined as follows: $V(\Xi) = V(M) \times \mathbf{Z}$ and $E(\Xi) = \bigcup_{i \in \mathbf{Z}} (E_i \cup X_i)$ where $E_i = \{(u,i)(v,i) \mid uv \in E(M)\}$ and $X_i = \{(u,i)(v,i+1) \mid (u,v) \in X\}$, $i \in \mathbf{Z}$. By M_i ($i \in \mathbf{Z}$) we will denote the subgraph induced on $V(M) \times \{i\}$. Clearly, each M_i is just a copy of M.

Given a graph G, we denote by $A = A(G)$ and $D = D(G)$ its *adjacency* and its *distance matrix*, respectively. The entry a_{uv} of A is equal to 1 if $uv \in E(G)$, and 0 otherwise. By $\tilde{A}$ we denote the matrix with entries $\tilde{a}_{uv} = a_{uv}$ if $a_{uv} \neq 0$ or $u = v$, and $\tilde{a}_{uv} = \infty$ otherwise. The entry d_{uv} of D is equal to $\mathrm{dist}_G(u,v)$, the length of a shortest path in G from u to v. If u and v are in distinct connected components of G, then $d_{uv} = \infty$.

When considering distance problems in graphs, it is useful to introduce a semiring over the extended non-negative integers $\mathbf{N}_0^* = \mathbf{N}_0 \cup \{\infty\}$ with operations min (as the addition) and + (as the multiplication). The matrix product over this semiring will be denoted by $\circ$. If A, B are square matrices of the same order k with entries in $\mathbf{N}_0^*$, then

$$(A \circ B)_{uv} = \min_{1 \le i \le k} (A_{ui} + B_{iv})\,. \tag{1}$$

For an extensive survey of results and applications concerning the above matrix product the interested reader is invited to consult [3, 4, 5, 13].

The distance matrix D of the graph G can be obtained from the matrix $\tilde{A}$ by computing its powers using the above product:

$$D = \underbrace{\tilde{A} \circ \tilde{A} \circ \cdots \circ \tilde{A}}_{n-1} = \tilde{A}^{n-1} \tag{2}$$

where n is the number of vertices of G. Instead of the power $n-1$, it suffices to take only $\mathrm{diam}(G)$ factors in (2).

Let $\Xi(M,X)$ be an infinite chain graph based on M where $|V(M)| = k$. Define the $k \times k$ *transition matrix* $T(X) = [t_{uv}]_{u,v \in V(M)}$ in the following way:

$$t_{uv} = \begin{cases} 1, & (u,v) \in X \\ \infty, & \text{otherwise.} \end{cases}$$

The following lemma, a reformulation of a result from [9], presents basic properties of partial distance matrices in infinite chain graphs.

Lemma 2.1 *Let $\Xi = \Xi(M,X)$ be an infinite chain graph and $k = |V(M)|$. Let D_0 be the $k \times k$ matrix with entries $(D_0)_{uv} = \mathrm{dist}_\Xi((u,0),(v,0))$. For $i > 0$, define $D_i = D_{i-1} \circ T(X) \circ D_0$. Then for each $j \in \mathbf{Z}$, the matrix D_i $(i = 0,1,\ldots)$ contains distances in Ξ between all pairs of vertices (u,j), $(v,j+i)$. More formally, $(D_i)_{uv} = \mathrm{dist}_\Xi((u,j),(v,j+i))$. Furthermore,*

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

Proof. Observe first that it is enough to prove the claim for $j = 0$. The proof is by induction on i. The base $i = 0$ is true by the definition of D_0. Suppose now that the claim holds for $i-1$, $i > 0$, and consider the equality

$$(D_i)_{uv} = \min_{1 \le w \le k} ((D_{i-1})_{uw} + (T(X) \circ D_0)_{wv})\,.$$

By the induction hypothesis, $(D_{i-1})_{uw}$ is the length of a shortest path between $(u,0)$ and $(w,i-1)$. Observe, finally, that $(T(X) \circ D_0)_{wv}$ is the length of a shortest path from $(w,i-1)$ to (v,i) such that the first edge of this path is of the form $(v,i-1)(v',i)$, where $(v,v') \in X$. Since every shortest path from $(u,0)$ to (v,i) uses such an edge, this implies the first part of the lemma.

The equality $D_{i+j} = D_i \circ D_j$ follows from $D_0 = D_0 \circ D_0$. $\square$

Let us remark that idempotency of D_0 also implies that

$$D_i = (D_1)^i, \quad i > 0\,.$$

With each infinite chain graph $\Xi = \Xi(M, X)$ we associate a *mixed graph* M_X containing directed and undirected edges. The graph M_X is defined as follows. The vertex set of M_X is the same as for M, $V(M_X) = V(M)$, while the edge set $E(M_X)$ consists of undirected edges $E(M)$ and directed edges X. Let Q be a walk in M_X where also the directed edges can be traversed in each direction. By $|Q|$ we denote the *length* of Q, i.e., the number of edges in Q. For each edge e in Q, its *weight* $w(e)$ (with respect to Q) is defined as 0 if e is undirected, 1 if e is traversed by Q in the direction consistent with its orientation, and -1 otherwise. The *weight* $w(Q)$ of Q is defined as

$$w(Q) = \sum_{e \in Q} w(e)\,.$$

It is easy to see that $\mathrm{dist}_\Xi((u,i),(v,j))$ equals the length of a shortest uv-walk in M_X whose weight is equal to $j - i$.

Proposition 2.2 *Let $\Xi = \Xi(M, X)$ be a connected infinite chain graph and $k = |V(M)| > 1$. Then there exist a spanning subgraph M' of M and a subset $X' \subseteq X$ such that the infinite chain graph $\Xi(M', X')$ is connected and*

$$|E(M'_{X'})| = |E(M')| + |X'| < k + \log_2 k\,.$$

Proof. It is easy to see that Ξ is connected if and only if the directed graph M_X is weakly connected and there exists a closed walk Q in M_X of weight $w(Q) = 1$. Let T be a spanning tree in M_X and let $r \in V(T)$ be an arbitrary fixed vertex of T. For $e = uv \in E(M_X) \backslash E(T)$, denote by C_e the closed walk in $T + e$ (called the *fundamental closed walk* of e) which consists of the path from r to u, followed by e and by the path from v to r in T. Clearly, $|w(C_e)| \le k$. Since the fundamental walks generate the fundamental group of M_X (with base vertex r), Q can be expressed as a concatenation of several fundamental closed walks. Therefore the greatest common divisor of the set of the weights of all fundamental walks equals 1. Let $\mathcal{C}$ be a minimal set of fundamental walks with the above property. To prove the lemma, it suffices to see that $|\mathcal{C}| < \log_2 k + 1$. Choose $C_0 \in \mathcal{C}$ such that $|w(C_0)|$ is as small as possible and let P be the set of primes dividing $|w(C_0)|$. Since $\gcd\{w(C) \mid C \in \mathcal{C}\} = 1$, for each prime $p \in P$ there exists $C(p) \in \mathcal{C}$ such that $w(C(p))$ is not divisible by p. By minimality of $\mathcal{C}$, it follows that $\mathcal{C} = \{C(p) \mid p \in P\} \cup \{C_0\}$. Since $|w(C_0)| < k$ and the product of primes in P is at least $2^{|P|}$, but not greater than $|w(\mathcal{C}_0)|$, we have $|P| < \log_2 k$. Therefore $|\mathcal{C}| \le |P| + 1 < \log_2 k + 1$.

Let $F \subseteq E(M_X) \backslash E(T)$ be the set of edges that corresponds to the walks in $\mathcal{C}$. The above arguments show that one can take the undirected edges of $E(T) \cup F$ as $E(M')$, while the directed edges in $E(T) \cup F$ determine X'. $\square$

Let us remark that we can always achieve $|E(M')| < k$, while $|X'| \le \log_2 k$ does not hold in general. Moreover, since the product of the first p primes grows much faster than 2^p (even faster than $p!$), the above proof in fact shows that $|E(M'_{X'})| = k + o(\log k)$.

Theorem 2.3 *Let $\Xi = \Xi(M, X)$ be a connected infinite chain graph and $k = |V(M)|$. Then for any $i, j \in \mathbf{Z}$ and $u, v \in V(M)$ we have*

$$\mathrm{dist}_{\Xi}((u,i),(v,j)) < k \cdot (4k + |i-j|)\,. \tag{3}$$

Proof. Without loss of generality we may assume that $i \le j$. Let T be a spanning tree in M_X and $e_1, \ldots, e_l$ the edges in $E(M_X) \backslash E(T)$. Denote by C_s the fundamental closed walk with respect to T and a root $v \in V(T)$ that is determined by e_s and let $w_s = w(C_s)$. Clearly, $|w_s| \le k$. Let P be the path in T from u to v. Since $\gcd(w_1, \ldots, w_l) = 1$, there exists a uv-walk Q of weight $j - i$ that is composed of P and some of the closed walks C_s (where each C_s can appear in Q several times in one or the other direction). Denote by Q_t $(1 \le t \le |Q|)$ the subwalk of Q consisting of the first t edges in Q. Since $w(Q) = j - i$, $|w(P)| < k$, and $|w_s| \le k$ $(1 \le s \le l)$, we may achieve by possible rearrangement of the order of the walks C_s in Q that for each t

$$-2k < w(Q_t) \le j - i + 2k\,.$$

This implies that there exists a path from (u,i) to (v,j) in Ξ that contains only vertices of $H = M_{i-2k+1} \cup \cdots \cup M_{j+2k}$. Since the subgraph of Ξ induced by H has at most $k \cdot (4k + j - i)$ vertices, (3) holds. $\square$

Roughly speaking, Theorem 2.3 states that

$$\mathrm{dist}_G((u,i),(v,j)) = \mathcal{O}(k^2 + k \cdot |i-j|)\,. \tag{4}$$

Let us now show by an example that the order of magnitude in (4) cannot be improved.

Example 1. Choose a positive integer k congruent 1 modulo 4, $k = 4l + 1$. Let M be the graph with $V(M) = \{1, \ldots, k\}$ and $E(M) = \emptyset$. Define

$$\begin{aligned} X &= \{(i, i+1) \mid 1 \le i \le 2l+1\} \cup \{(i, i-1) \mid 2l+3 \le i \le 3l+1\} \\ &\quad \cup \{(i, i+1) \mid 3l+2 \le i \le 4l\} \cup \{(l+1, 3l+1), (l+1, 3l+2)\} \end{aligned}$$

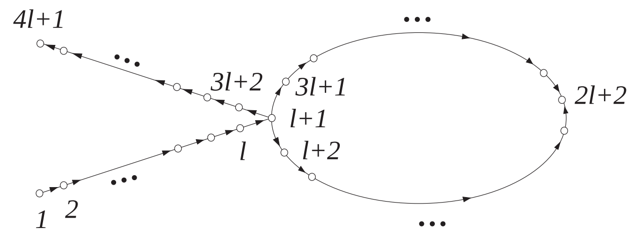


Figure 1: The mixed graph M_X of $\Xi(M, X)$.

and set $\Xi = \Xi(M, X)$. The associated mixed graph M_X is shown in Figure 1.

Since the weight of the cycle in M_X is equal to ± 1, it is easy to see that

$$\mathrm{dist}_\Xi((1,0),(k,i)) = \frac{k-1}{2} + \frac{k+1}{4} \cdot |2i - k + 1|$$

and

$$\mathrm{dist}_\Xi((1,0),(l+1,i)) = \frac{k-1}{4} + \frac{k+1}{8} \cdot |4i - k + 1| \,.$$

Finally, observe that for each k and i, the larger of the above distances is of the same order of magnitude as the upper bound in (4).

The above construction can be extended to the cases when k is not congruent to 1 modulo 4. $\square$

It can be shown that for large enough indices l matrices D_l have a special structure that enables us to compute them efficiently. The following proposition is a variant of the "cyclicity" theorem for the "tropical" semiring $(\mathbf{N}_0^*, \min, +)$, see, e.g., [3, Theorem 3.112]. By a constant matrix we mean a matrix with all entries equal.

Proposition 2.4 *Let $\Xi = \Xi(M, X)$ be a connected infinite chain graph, $k = |V(M)|$, and $K = \max\{(D_0)_{uv} \mid u, v \in V(M)\}$. Then there is an index $q \le (2K+1)^{k^2}$ such that $D_q = D_p + C$ for some index $p < q$ and some constant matrix C. Let $P = q - p$. Then for every $i \ge p$ and every $j \ge 0$ we have*

$$D_{i+jP} = D_i + jC \,.$$

Proof. For $l \ge 0$, let $D'_l = D_l - (D_l)_{11} J$ where J is the matrix with all entries equal to 1. Since the difference between any two elements of D_l cannot be greater than $2K$, there are indices $p < q \le (2K+1)^{k^2}$ such that $D'_p = D'_q$. This proves the first part of the proposition.

The equality $D_{i+jP} = D_i + jC$ follows from the fact that for arbitrary matrices A, B and a constant matrix C we have $(A + C) \circ B = A \circ B + C$. $\square$

Let us remark that the matrix C of Proposition 2.4 can be interpreted in terms of "eigenvalues" of D_1 with respect to the matrix product over the semiring $(\mathbf{N}_0^*, \min, +)$. The reader is referred to [3, 5] for more details.

The bound on q in Proposition 2.4 is far from being optimal. Our examples in Section 5 show that p and P are usually much smaller.

3 Fasciagraphs and rotagraphs

A subgraph of $\Xi(M,X)$ induced on $V(M)\times\{1,\ldots,n\}$ is called a *fasciagraph* and denoted by $\Xi_n(M,X)$. The *rotagraph* $\Xi_n^\circ(M,X)$ is obtained from $\Xi(M,X)$ by identifying vertices (v,i) and $(v,i+n)$ $(i \in \mathbf{Z}, v \in V(M))$. Alternatively, the fasciagraph $\Xi_n(M,X)$ can be obtained by taking n disjoint copies $M_1,\ldots,M_n$ of the graph M, and for $i=1,\ldots,n-1$ and for each $(u,v) \in X$, adding the edge $u_i v_{i+1}$ where $u_i \in V(M_i)$, $v_{i+1} \in V(M_{i+1})$ are copies of u and v, respectively. We can think of a rotagraph $\Xi_n^\circ(M,X)$ in the same way except that we also add edges $u_n v_1$ between M_n and M_1, $(u,v) \in X$.

Notice that the Cartesian product of M and the path P_n (M and the cycle C_n) is a special case of the fasciagraph (rotagraph) where $X = id$. Similarly, the direct, the strong, and several other products [1, 6] of M and P_n or C_n are special cases of fascia and rotagraphs.

We obtain partial distance matrices $D_{i,j}$ and $D_{i,j}^\circ$ containing distances in Ξ_n and Ξ_n° (respectively) between vertices of M_i and M_j $(1 \le i \le n, 1 \le j \le n)$ similarly as for the infinite chain graph. Because of circular symmetry of Ξ_n°, it is clear that $D_{i,j}^\circ$ depends only on $(j-i) \bmod n$. (The same property does not hold for fasciagraphs.) Also,

$$D_{j,i} = D_{i,j}^{\mathrm{T}} \quad \text{and} \quad D_{j,i}^\circ = {D_{i,j}^\circ}^{\mathrm{T}}.$$

Most of the partial distance matrices $D_{i,j}$ and $D_{i,j}^\circ$ can be obtained from the matrices D_l of the corresponding infinite chain graph as follows:

Proposition 3.1 *Suppose that the infinite chain graph $\Xi = \Xi(M,X)$ is connected. Let $k = |V(M)|$ and $n \in \mathbf{N}$. Denote by K the maximum element of D_0. Then $K < 4k^2$. Moreover:*

- *(a) If $K/2 < i \le j < n - K/2 + 1$, then $D_{i,j} = D_{j-i}$.*
- *(b) If $n \ge K$ and $0 \le j - i < n$, then $D_{i,j}^\circ = \min\{D_{j-i}, D_{n-j+i}^{\mathrm{T}}\}$ where the minimum is taken elementwise. If also $j - i \le n/2 - K$, then $D_{i,j}^\circ = D_{j-i}$.*

Proof. Theorem 2.3 implies that $K < 4k^2$. By the definition of K, for every pair of vertices $(u,i),(v,j) \in V(\Xi)$, $i \le j$, all shortest paths between (u,i) and (v,j) contain only vertices of $M_{i-\lfloor K/2\rfloor},\ldots,M_{j+\lfloor K/2\rfloor}$. This implies (a). To justify (b), observe that in a rotagraph $\Xi_n^\circ = \Xi_n^\circ(M,X)$ where $n \geq K$, there is always a shortest path between (u,i) and (v,j) in Ξ_n° that corresponds to either a path between (u,i) and (v,j) in Ξ, or a path between (u,i) and $(v,j-n)$ in Ξ. (Note that when $n < K$, all shortest paths between (u,i) and (v,j) in Ξ_n° could correspond to paths between (u,i) and, e.g., $(v,j+n)$ in Ξ.) The length of a shortest path of the first type is equal to $(D_{j-i})_{uv}$, while a shortest path of the second type has length $(D_{n-j+i})_{vu}$. This proves the first part of (b). If also $j-i \leq \frac{n}{2}-K$, then $(n-j+i)-(j-i) \geq 2K$, which finally gives $(D_{j-i})_{uv} \leq (D_{n-j+i})_{vu}$. □

One can apply Proposition 3.1 in problems related to distances in polygraphs. An example of such an approach is presented in the next section.

In [9] we treated the isometric case when (each copy of) M is an isometric subgraph of $\Xi(M,X)$, i.e., the distance matrix of M is equal to D_0. (More generally, a subgraph H of G is an *isometric* subgraph if for any two vertices $u,v \in V(H)$, the distance from u to v in H is equal to their distance in G.) In the isometric case we have

$$D_{i,j} = D_{j-i}$$

for all $1 \leq i \leq j \leq n$. Similarly,

$$D_{i,j}^\circ = D_{j-i}$$

for all $1 \leq i \leq j \leq n$ such that $j-i \leq \lfloor\frac{n}{2}\rfloor - k + 1$.

If i and j are not within the intervals requested in Proposition 3.1, the matrices $D_{i,j}$ and D_{j-i} do not always coincide. Next we prove that their entries cannot differ too much.

Lemma 3.2 *Suppose that $\Xi(M,X)$ is an infinite chain graph and let K be the maximum element of D_0. Suppose that $\Xi_n = \Xi_n(M,X)$ is connected. If $1 \leq i \leq j \leq n$ and $u,v \in V(M)$, then*

$$(D_{j-i})_{uv} \leq (D_{i,j})_{uv} \leq (D_{j-i})_{uv} + K(k+2)\,.$$

Proof. The first inequality is obvious. For the second one, we may assume that $n > K$. Let $L_1 = \lfloor K/2\rfloor + 1$ and $L_2 = n - \lfloor K/2\rfloor$. Suppose first that $1 \leq i < L_1$ and $L_2 < j \leq n$. Let P be a shortest path in $\Xi(M,X)$ from (u,i) to (v,j). Let P' be a segment of P from a vertex (u',L_1) to (v',L_2). Since $n > K$, P' exists. Let P_1 be a shortest path in Ξ_n from (u,i) to some vertex (u'',L_1). Then $|P_1| \leq kK/2$. Similarly, if P_2 is a shortest path in Ξ_n from a vertex (v'',L_2) to (v,j), then $|P_2| \leq kK/2$. Since there is a path P_1' in $\Xi(M,X)$ from (u'',L_1) to (u',L_1) of length at most K, such a path exists also in Ξ_n by

Proposition 3.1(a). Similarly we get a path P_2' from (v'', L_2) to (v', L_2). Paths P_1, P_1', P', P_2', P_2 show that the distance in Ξ_n from (u,i) to (v,j) is at most $K(k+2)+|P|$.

The cases where $1 \le i < L_1$ and $1 \le j < L_1$ (or $L_1 \le j \le L_2$) are proved similarly. (One even gains a factor of 2 since $|P_1|+|P_2| \le kK/2$ and only one path between vertices of M_{L_1} is needed.) In cases when $i > L_2$ we get the same bounds by symmetry. In all other cases, Proposition 3.1(a) applies. $\square$

It may happen that $\Xi_n^\circ(M,X)$ is connected and that $\Xi(M,X)$ is disconnected. For example, if $M = \overline{K}_2$, $X = \{(1,2),(2,1)\}$, and n is odd. On the other hand, the connectivity of $\Xi(M,X)$ always implies the connectivity of $\Xi_n^\circ(M,X)$. It is interesting that for fasciagraphs, the reverse statements hold: $\Xi_n(M,X)$ being connected for some $n \ge 1$ implies that $\Xi(M,X)$ is connected (recall that $X \ne \emptyset$), while the connectivity of $\Xi(M,X)$ does not yield connectivity of $\Xi_n(M,X)$. Hence, the connectivity of $\Xi(M,X)$ and $\Xi_n(M,X)$ is a local property (by Theorem 2.3), but the connectivity of $\Xi_n^\circ(M,X)$ is not a local property.

4 The Wiener index

The Wiener index $W(G)$ of G is the sum of all distances in G:

$$W(G) = \frac{1}{2} \sum_{u \in V(G)} \sum_{v \in V(G)} d_{uv}\,. \tag{5}$$

This index was introduced in 1947 [15], when Wiener observed a good correlation between the boiling points of paraffins and $W(G)$ of the corresponding molecular graphs.

Although it was the first topological index studied, even today it is a widely employed graph theoretical descriptor [14]. For more information on the applicability of the Wiener index the reader is advised to consult other articles in this volume. The Wiener index of polymer molecular graphs that correspond to our notion of polygraphs has been studied in [7, 11]. Regarding the computation of the Wiener index see [8, 12].

In [9], an observation that the distance matrices of polygraphs blocks which can be computed efficiently, was used to give algorithms for computing the Wiener index of polygraphs. In particular, if the polygraph is a fascia or rotagraph, formulas for the Wiener index of infinite families $\Xi_n(M,X)$ and $\Xi_n^\circ(M,X)$ can be derived. In [9], an explicit formula for the Wiener index of fasciagraphs (and rotagraphs) is given in case when M is an isometric subgraph of the polygraph.

In the sequel, we shall express the Wiener index by using the sums of distances between all pairs of vertices in M_0 and M_i. Hence we set for each integer $i > 0$:

$$s_i = \sum_{u \in V(M)} \sum_{v \in V(M)} (D_i)_{uv}$$

and

$$s_0 = \frac{1}{2} \sum_{u \in V(M)} \sum_{v \in V(M)} (D_0)_{uv} \, .$$

Given a connected infinite chain graph $\Xi(M, X)$, denote by p and q, $0 \leq p < q$, the smallest integers such that $D_q = D_p + C$, where C is a constant matrix. Recall that Proposition 2.4 guarantees that such integers do exist. The numbers p and $P = q - p$ are called the *preperiod* and the *period* of $\Xi(M, X)$, respectively.

Theorem 4.1 *[9] Let M be a connected graph with k vertices and suppose that each copy of M is an isometric subgraph of $\Xi_n(M, X)$. Let p, P, and C be defined as above and let all entries of C be equal to c. Set $m = \lfloor (n-p)/P \rfloor$ and let $r = n - 1 - mP$. If $n \geq p$, then*

$$\begin{aligned} W(\Xi_n(M, X)) &= \sum_{i=0}^{r} (n-i) s_i + m \sum_{i=1}^{P} \Big(n - r - \frac{(m-1)P}{2} - i \Big) s_{r+i} \\ &\quad + \frac{k^2 c (m-1) m P}{2} \Big(n - r - \frac{(2m-1)P}{3} - \frac{P+1}{2} \Big) \, . \end{aligned}$$

Let us remark that for $n \geq p$, Theorem 4.1 implies that for each congruence class modulo the period P, the Wiener index $W(\Xi_n(M, X))$ is a cubic polynomial in n. More precisely, one can show that all these polynomials for distinct congruence classes differ only in the constant term, all other coefficients are independent of n mod P (see Example 3).

Theorem 4.1 also shows that in order to obtain the Wiener index of a given fasciagraph with isometric monographs, it suffices to compute only the matrices $D_0, \ldots, D_{r+P}$, where P and r are defined above. 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.

The results of Theorem 4.1 can also be extended to the case when monographs are not isometric subgraphs of the fasciagraph. In such a case the first and the last $\lfloor \frac{K}{2} \rfloor$ monographs have to be considered separately (where K is the maximum element of D_0), and this additional requirement increases the complexity of the obtained formula. Therefore we decided to present only asymptotic results.

Corollary 4.2 *Let $\Xi_n(M,X)$ be a connected fasciagraph. Let k, p, P, c, m, and r be defined as in Theorem 4.1 and let K be the maximum element of D_0. Then*

$$\begin{aligned} W(\Xi_n(M,X)) &= \sum_{i=0}^{r}(n-i)s_i + m\sum_{i=1}^{P}\Big(n-r-\frac{(m-1)P}{2}-i\Big)s_{r+i} \\ &\quad + \frac{k^2c(m-1)mP}{2}\Big(n-r-\frac{(2m-1)P}{3}-\frac{P+1}{2}\Big) \\ &\quad + \mathcal{O}(K^2k^3n)\,. \end{aligned}$$

Proof. Denote by W_n the sum of all distances in $\Xi(M,X)$ between distinct vertices of $M_1 \cup \cdots \cup M_n$ and set $W = W(\Xi_n(M,X))$. A calculation used in obtaining the proof of Theorem 4.1 in [9] shows that for $n \geq p$, the sum in Theorem 4.1 is equal to W_n. Therefore it remains to show that

$$W - W_n = \mathcal{O}(K^2k^3n)\,.$$

Given i and j, $1 \leq i \leq j \leq n$, let

$$\Delta_{i,j} = \sum_{u,v\in V(M)}\Big((D_{i,j})_{uv} - (D_{j-i})_{uv}\Big)\,.$$

Note that $\Delta_{i,j} \geq 0$. By the definition,

$$W - W_n \leq \sum_{i=1}^{n}\sum_{j=i}^{n}\Delta_{i,j}\,.$$

For $K/2 < i \leq j < n-K/2+1$, Proposition 3.1(a) implies that $\Delta_{i,j} = 0$. On the other hand, when $i \leq K/2$ or $j \geq n-K/2+1$, Lemma 3.2 gives $\Delta_{i,j} \leq Kk^2(k+2)$. Therefore

$$W - W_n \leq \sum_{i=1}^{\lfloor K/2\rfloor}\sum_{j=i}^{n}\Delta_{i,j} + \sum_{j=n-\lfloor K/2\rfloor+1}^{n}\ \sum_{i=\lfloor K/2\rfloor+1}^{j}\Delta_{i,j} \leq K^2k^2(k+2)n\,,$$

which proves the corollary. $\square$

A companion of Theorem 4.1 for rotagraphs proved in [9] for isometric monographs yields a similar result for the Wiener index of rotagraphs.

Corollary 4.3 *Suppose that $\Xi(M,X)$ is a connected infinite chain graph and let k, p, P, and c be defined as in Theorem 4.1. Set $N = \lfloor\frac{n}{2}\rfloor - K$, $m = \lfloor(N+1-p)/P\rfloor$, $r = N - mP$, and let K be the maximum element of D_0. If $N+1 \geq p$, then*

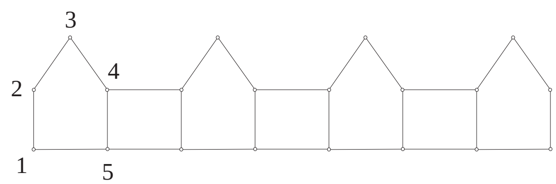
$$W(\Xi_n^\circ(M,X)) = \frac{n}{2}\cdot\Big(2\sum_{i=0}^{r}s_i + 2m\sum_{i=1}^{P}s_{r+i} + k^2c(m-1)mP + \sum_{i=N+1}^{n-N-1}s_i^\circ\Big)\,,$$

where s_i° denotes the sum of all elements in the matrix $D_{0,i}^\circ$.

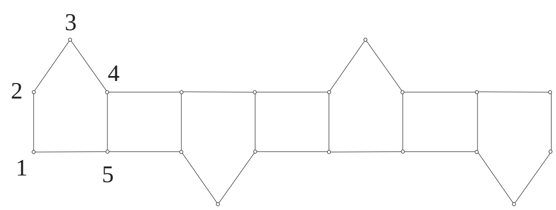
Observe that the entries of $D^{\circ}_{0,i}$ can be efficiently computed since $D^{\circ}_{0,i} = \min\{D_i, D^{\mathrm{T}}_{n-i}\}$. Similarly to the case of fasciagraphs one can show that n large enough for each congruence class modulo $2P$, the Wiener index of a rotagraph is a cubic polynomial in n.

5 Examples

We conclude by four examples which should serve as a demonstration of the method from Section 4.



(a)



(b)

Figure 2: The graphs of Examples 2 and 3.

Example 2. Consider a fasciagraph obtained by taking n 5-cycles C_5 as the monographs and connected as in Figure 2(a) for the case $n = 4$. The matrices $D_0 = D(G)$ and $T(X)$ are

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

while the matrices D_1 and D_2 are equal to

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

and the matrices D_3 and D_4 are equal to

$$\begin{bmatrix} 6 & 7 & 8 & 8 & 7 \\ 7 & 8 & 9 & 9 & 8 \\ 7 & 8 & 9 & 9 & 8 \\ 6 & 7 & 8 & 8 & 7 \\ 5 & 6 & 7 & 7 & 6 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 8 & 9 & 10 & 10 & 9 \\ 9 & 10 & 11 & 11 & 10 \\ 9 & 10 & 11 & 11 & 10 \\ 8 & 9 & 10 & 10 & 9 \\ 7 & 8 & 9 & 9 & 8 \end{bmatrix}.$$

Therefore we have $k = 5$, $p = 3$, $q = 4$, $P = 1$, $c = 2$, $m = n-3$, $r = 2$, $s_0 = 15$, $s_1 = 73$, $s_2 = 131$, and $s_3 = 185$. Applying Theorem 4.1 we get

$$\begin{aligned} W &= ns_0 + (n-1)s_1 + (n-2)s_2 + \frac{1}{2}(n-3)(n-2)s_3 \\ &\quad + \frac{25}{3}(n-4)(n-3)(n-2) \\ &= \frac{1}{6}(50n^3 + 105n^2 - 161n + 120)\,. \end{aligned}$$

$\square$

Example 3. Take a fasciagraph obtained by taking n 5-cycles C_5 as the monographs which are connected as in Figure 2(b) for the case $n = 4$. In this case $X = \{(4,1),(5,2)\}$. The matrices $D_0 = D(G)$ and D_1 are

$$\begin{bmatrix} 0 & 1 & 2 & 2 & 1 \\ 1 & 0 & 1 & 2 & 2 \\ 2 & 1 & 0 & 1 & 2 \\ 2 & 2 & 1 & 0 & 1 \\ 1 & 2 & 2 & 1 & 0 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 3 & 2 & 3 & 4 & 4 \\ 3 & 3 & 4 & 5 & 4 \\ 2 & 3 & 4 & 4 & 3 \\ 1 & 2 & 3 & 3 & 2 \\ 2 & 1 & 2 & 3 & 3 \end{bmatrix},$$

while the matrices D_2 and D_3 are equal to

$$\begin{bmatrix} 5 & 5 & 6 & 7 & 6 \\ 6 & 5 & 6 & 7 & 7 \\ 5 & 4 & 5 & 6 & 6 \\ 4 & 3 & 4 & 5 & 5 \\ 4 & 4 & 5 & 6 & 5 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 8 & 7 & 8 & 9 & 9 \\ 8 & 8 & 9 & 10 & 9 \\ 7 & 7 & 8 & 9 & 8 \\ 6 & 6 & 7 & 8 & 7 \\ 7 & 6 & 7 & 8 & 8 \end{bmatrix}.$$

The matrix D_4 is equal to $D_2 + C$, where C has all entries equal to 5. Hence we have $k = 5$, $p = 2$, $q = 4$, $P = 2$, $c = 5$, $m = \lfloor \frac{n}{2} \rfloor - 1$, $r = 1 + n \bmod 2$, $s_0 = 15$, $s_1 = 73$, $s_2 = 131$, and $s_3 = 194$. By Theorem 4.1 we get

$$W = \begin{cases} \frac{1}{24}(250n^3 + 75n^2 + 134n - 99), & n \text{ odd} \\ \frac{1}{24}(250n^3 + 75n^2 + 134n - 96), & n \text{ even.} \end{cases}$$

□

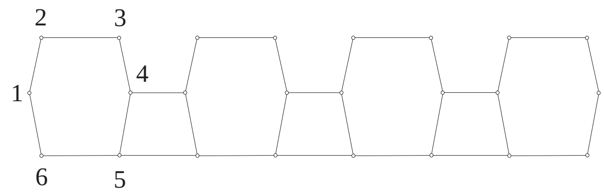


Figure 3: The graph of Example 4.

Example 4. As our next example, consider first the fasciagraphs obtained by taking 6-cycles C_6 as the monographs and connected as in Figure 3 for the case $n = 4$. Here $X = \{(4,1),(5,6)\}$. The matrices $D_0 = D(G)$ and D_1 are

$$\begin{bmatrix} 0 & 1 & 2 & 3 & 2 & 1 \\ 1 & 0 & 1 & 2 & 3 & 2 \\ 2 & 1 & 0 & 1 & 2 & 3 \\ 3 & 2 & 1 & 0 & 1 & 2 \\ 2 & 3 & 2 & 1 & 0 & 1 \\ 1 & 2 & 3 & 2 & 1 & 0 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 4 & 5 & 6 & 5 & 4 & 3 \\ 3 & 4 & 5 & 6 & 5 & 4 \\ 2 & 3 & 4 & 5 & 4 & 3 \\ 1 & 2 & 3 & 4 & 3 & 2 \\ 2 & 3 & 4 & 3 & 2 & 1 \\ 3 & 4 & 5 & 4 & 3 & 2 \end{bmatrix},$$

while the matrices D_2 and D_3 are equal to

$$\begin{bmatrix} 6 & 7 & 8 & 7 & 6 & 5 \\ 7 & 8 & 9 & 8 & 7 & 6 \\ 6 & 7 & 8 & 7 & 6 & 5 \\ 5 & 6 & 7 & 6 & 5 & 4 \\ 4 & 5 & 6 & 5 & 4 & 3 \\ 5 & 6 & 7 & 6 & 5 & 4 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 8 & 9 & 10 & 9 & 8 & 7 \\ 9 & 10 & 11 & 10 & 9 & 8 \\ 8 & 9 & 10 & 9 & 8 & 7 \\ 7 & 8 & 9 & 8 & 7 & 6 \\ 6 & 7 & 8 & 7 & 6 & 5 \\ 7 & 8 & 9 & 8 & 7 & 6 \end{bmatrix}.$$

As $D_3 - D_2 = 2J$, we have $k = 6$, $p = 2$, $q = 3$, $P = 1$, $c = 2$, $m = n - 2$, $r = 1$, $s_0 = 27$, $s_1 = 126$, and $s_2 = 216$. By Theorem 4.1 we get

$$W(\Xi_n(M,X)) = 12n^3 + 36n^2 - 39n + 18\,.$$

To compute the Wiener index of the rotagraphs $\Xi_n^\circ(M,X)$, some additional work is needed. Since $D_i = D_2 + 2(i-2)J$, $i>1$, and the absolute value of the largest element of $D_2 - D_2^T$ is equal to 2, we have

$$\begin{aligned}
D_{0,i}^\circ &= \min\{D_i, D_{n-i}^T\} = \min\{D_2 + 2(i-2)J, D_2^T + 2(n-i-2)J\} \\
&= \begin{cases} D_i, & 1 < i < \frac{n}{2} \\ \min\{D_i, D_i^T\}, & i = \frac{n}{2} \\ D_{n-i}^T, & \frac{n}{2} < i < n-1. \end{cases}
\end{aligned}$$

In particular,

$$s_i^\circ = \begin{cases} 72i + 72, & 1 < i < \frac{n}{2} \\ 72i + 54, & i = \frac{n}{2} \\ 72(n-i) + 72, & \frac{n}{2} < i < n-1. \end{cases}$$

Finally, for $n \geq 8$, Corollary 4.3 implies that

$$W(\Xi_n^\circ(M,X)) = 9n^3 + 36n^2 - 36n\,. \tag{6}$$

Let us remark that (6) is in fact true for all $n \geq 3$. □

Example 5. Let $M = P_k$ be a path of order k. Label the vertices of M by $1,\ldots,k$ in order as they appear on M and set $X = \{(1,1),(k,1)\}$. Observe that in this case the monographs are not isometric subgraphs of $\Xi(M,X)$. Since 1 is the only vertex of M that has a neighbor in the previous monograph, we have

$$(D_i)_{uv} = \min\{u, k+1-u\} + i - 1 + \min\{v-1, k+2-v\}$$

for $i > 0$. Moreover, for $u \leq v$,

$$(D_0)_{uv} = \min\{v-u, k+1-(v-u)\}\,.$$

Therefore $p=1$, $q=2$, $P=1$, and $c=1$. Let $\kappa = \lfloor (k+1)^2/4 \rfloor$. A short calculation shows that $s_0 = (k-1)\kappa/2$ and $s_i = k(2\kappa - 1) + k^2(i-1)$, $i > 0$. Since our example has a very simple structure, $D_{i,j} = D_{j-i}$ for $1 \leq i \leq j < n$ and $(D_{i,n})_{uv} = \min\{u, k+1-u\} + (n-i) + v - 2$ for $0 < i < n$ and $u,v \in V(M)$. Hence, the Wiener index of the fasciagraphs $\Xi_n(M,X)$ can be expressed as

$$\begin{aligned}
W &= \sum_{i=1}^{n-1}(n-i)s_{i-1} + \sum_{i=1}^{n-1}\sum_{u,v\in V(M)}(D_{i,n})_{uv} + \frac{(k-1)k(k+1)}{6} \\
&= \frac{1}{6}\Big(k^2n^3 + (6\kappa - 3k - 3)kn^2 + (3k^3 - 9k\kappa - k^2 - 3\kappa + 9k)n + 3k\kappa - 2k^3 + 3k^2 + 3\kappa - 7k\Big) \\
&= \begin{cases} \frac{1}{24}(4k^2n^3 + 6k(k^2-1)n^2 + (3k^3 - 25k^2 + 21k - 3)n - 5k^3 + 21k^2 - 19k + 3), & n \text{ odd} \\ \frac{1}{24}(4k^2n^3 + 6k(k^2-2)n^2 + (3k^3 - 25k^2 + 30k)n - 5k^3 + 21k^2 - 22k), & n \text{ even.} \end{cases}
\end{aligned}$$

Comparing W to the expression

$$W_n = \frac{1}{6}\Big(k^2n^3 + (6\kappa - 3k - 3)kn^2 + (-3k\kappa + 2k^2 - 3\kappa + 3k)n\Big)$$

from Theorem 4.1 we see that the order of magnitude of the difference

$$W - W_n = \frac{1}{6}\Big(3(k^2 - 2\kappa - k + 2)kn - 2k^3 + 3k\kappa + 3k^2 + 3\kappa - 7k\Big) = \mathcal{O}(k^3n)$$

is as claimed by Corollary 4.2. $\square$

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