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The Szeged index of fasciagraphs[1]

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Abstract

Let $G^{(n)}$ be a graph which is obtained from a path P_n by replacing each vertex by a fixed graph G and replacing each edge by a fixed set of edges joining the corresponding copies of G. A matrix approach to the computation of distance-based invariants which gives a general procedure to obtain closed-form expressions (depending on n) for such invariants of $G^{(n)}$ was given in Ref. 11. Here we illustrate how to apply the approach to the Szeged index (first defined in Ref. 6), a graph invariant which has recently received considerable attention in chemical graph theory.

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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 efficient procedures for computing several graph invariants.[12] It was shown in Ref. 10 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 Ref. 11 the same approach was used to study a general class of distance related graph invariants. A general theory of such invariants on infinite chain graphs was initiated and the results were illustrated on a well-known distance-related graph invariant, the Wiener index.[15] In this paper we show how the same approach can be applied to another recently introduced distance-related graph invariant, the Szeged index.[6]

The structure of the paper is as follows. In Section 2 some definitions and statements on distances in infinite chain graph are given. Special results for fasciagraphs are recalled in Section 3. In Section 4 the general theory on distance-related invariants is applied to the Szeged index. The method is illustrated on several examples in Section 5.

2 Distances in infinite chain graphs

In this section we recall the definition of infinite chain graphs and some results on distance matrices in such graphs. The key observation is Proposition 2.2 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. For brevity, we will use notation $uv = (u,v) \in X$, analogous to notation used for edges. (In examples, we again prefer (11,12) to 1112 for clarity.) Denote by **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 $X_i = \{(u,i)(v,i+1) \mid uv \in X\}$, $i \in \mathbf{Z}$. 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. An example where $M = C_6$ is the 6-cycle and $X = \{(4,1),(5,6)\}$ is shown in Figure 1.

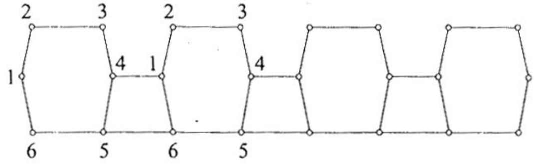


Figure 1: A part of an infinite chain graph based on C_6.

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 $\tilde{a}_{uv} = 0$ if $u = v$, $\tilde{a}_{uv} = 1$ if $uv \in E(G)$, 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 addition) and + (as 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 reader is invited to consult Refs. 3–5, 14.
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) (where $\mathrm{diam}(G)$ is the diameter of the graph G, i.e., the maximum over all distances between pairs of vertices of G).
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 Ref. 10, 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,*

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

Let us remark that idempotency of D_0 also implies that

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

It can be shown that for large enough values of index ℓ matrices D_ℓ have special structure that enables us to compute them efficiently. The following proposition, stated as Proposition 2.4. in Ref. 11, is a variant of the "cyclicity" theorem for the "tropical" semiring $(\mathbf{N}_0^*, \min, +)$, see, e.g., Ref. 3, Theorem 3.112. By a constant matrix we mean a matrix with all entries equal.

Proposition 2.2 *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 are indices p, q, $0 \le p < q \le (2K+1)^{k^2}$, such that $D_q = D_p + C$, where C is a constant matrix. Let $P = q - p$. Then for every $i \ge p$ and every $j \ge 0$ we have*

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

The (minimal values of) indices p and P are called ***preperiod*** and ***period*** of the infinite chain graph Ξ, respectively. Let us remark that the matrix C of Proposition 2.2 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 Refs. 3,5 for more details.
The upper bound on q in Proposition 2.2 is far from being optimal. Our examples in Section 5 show that p and P are usually much smaller.

3 Fasciagraphs

A subgraph of $\Xi(M, X)$ induced on $V(M) \times \{1, \ldots, n\}$ is called a *fasciagraph* and denoted by $\Xi_n(M, X)$. 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 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. Notice that the Cartesian product of M and the path P_n is a special case of the fasciagraph where $X = id$. Similarly, the direct, the strong, and several other products[1] of M and P_n are special cases of fasciagraphs.
We obtain partial distance matrices $D_{i,j}$ containing distances in Ξ_n 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. Note that in general $D_{i,j}$ does not depend only on $(j-i) \bmod n$. Also, $D_{j,i} = D_{i,j}^T$. Most of the partial distance matrices $D_{i,j}$ can be obtained from the matrices D_ℓ of the corresponding infinite chain graph as follows (see Ref. 11):

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: If $K/2 < i \le j < n - K/2 + 1$, then $D_{i,j} = D_{j-i}$.*

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 Ref. 10 (as well as in this paper) we treat 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

$$D_{i,j} = D_{j-i} \tag{3}$$

for all $1 \le i \le j \le n$.

4 The Szeged index

The Szeged index Sz is a recently proposed structural descriptor, based on the distances of vertices in a molecular graph.[6] As one can expect,[9] it resembles the Wiener index,[15] the first and still perhaps the most studied topological index. For reasons to introduce the Szeged index and for its basic properties see Refs. 6,9. For general graphs, the Szeged index can be computed in $O(|V| \cdot |E|)$ time.[17] On some special families of graphs it is possible to use faster algorithms. For example, an algorithm for computing the Szeged index of benzenoid hydrocarbons was given in Ref. 7. Since the Wiener and Szeged index

coincide on trees, the linear algorithm can be used for computing the Szeged index of trees.[13] For more references, see Ref. 8.
We know that for polygraphs the computation of the Szeged index can be done even faster than in linear time because the Szeged index is a distance based invariant.[11] Moreover, the method derived in Refs. 10–12 can be used to find closed-form expressions for the Szeged index of families of fasciagraphs. In this paper we show how the method can be applied in the case of the Szeged index. Some examples are given in the next section. The same ideas can also be used to find the Szeged index of families of rotagraphs (where *rotagraph* is a graph obtained from a fasciagraph $\Xi_n = \Xi_n(M, X)$ by adding edges also between the last and the first copy of M in Ξ_n).
Let us recall the definition of the Szeged index. If $u, v \in V(G)$ are vertices of G, let $\mathcal{N}(u, v)$ denote the set of vertices of G which are closer to u than to v, i.e.,

$$\mathcal{N}(u, v) = \{w \in V(G) \mid \mathrm{dist}_G(u, w) < \mathrm{dist}_G(v, w)\}.$$

Furthermore, let $n(u, v) = |\mathcal{N}(u, v)|$. Then we define the Szeged index $Sz(G)$ as

$$Sz(G) = \sum_{uv \in E(G)} n(u, v) \cdot n(v, u)$$

where the sum runs over all edges of G.
Suppose that $G = \Xi(M, X)$ is an infinite chain graph and let $u, v \in V(G)$. Then we define similarly as above $n^{(i)}(u, v)$ to be the number of vertices w in the monograph $M_i = M \times \{i\}$, for which $\mathrm{dist}_G(u, w) < \mathrm{dist}_G(v, w)$. The same notation will be used in the fasciagraphs $\Xi_n(M, X)$.

Proposition 4.1 *Let $\Xi = \Xi(M, X)$ be an infinite chain graph and let p and P be defined as in Proposition 2.2. Suppose that $x = (u, 0), y = (v, d) \in V(\Xi)$, where $d \geq 0$. Then we have*

$$n^{(i+P)}(x, y) = n^{(i)}(x, y) \qquad for \quad i \geq p + d$$

and

$$n^{(-j-P)}(x, y) = n^{(-j)}(x, y) \quad for \quad j \geq p\,.$$

Proof. Observe first that for $i \geq d$ the number $n^{(i)}(x, y)$ is equal to the number of negative entries in the vector obtained as a difference between the u-th row of D_i and the v-th row of D_{i-d}. When $i \geq p + d$, by Proposition 2.2 we have $D_{i+P} = D_i + C$ and $D_{i-d+P} = D_{i-d} + C$ for some constant matrix C, which implies the first equality.
Similarly, for $j \geq 0$ the number $n^{(-j)}(x, y)$ is equal to the number of negative entries in the vector obtained as a difference between the u-th column of D_j and the v-th column of D_{j+d}. When $j \geq p$, Proposition 2.2 applies and also the second equality follows. □

Note that when $e = xy$ is an edge of $\Xi(M, X)$, we have $d = -1$, 0 or 1.
In general it might happen that the (minimal) period (and preperiod) of the sequence $n^{(i)}(x, y)$ $(i \geq 0)$ is smaller than P (and p, respectively). But it is always the case that the period of this sequence divides P. It is also possible that the period of $n^{(i)}(x, y)$ $(i \geq 0)$ is not equal to the period of $n^{(-j)}(x, y)$ $(j \geq 0)$. (See examples in the last section.)
The proof of Proposition 4.1 also shows how to determine the values of $n^{(i)}(x, y)$ when the distance matrices D_i $(i = 0, 1, 2, \ldots)$ are known. In particular, this can be efficiently applied in computer-aided calculations.

When applying the above results to fasciagraphs, we have to consider separately the monographs close to the two ends of the fasciagraph $\Xi_n(M, X)$. If there exists a copy of M that is not an isometric subgraph of $\Xi_n(M, X)$, then additional difficulties arise since (3) need not always hold. This does not happen in the isometric case which we assume henceforth (see the definition after Proposition 3.1).
Let $\Xi_n = \Xi_n(M, X)$ be a fasciagraph such that each copy of M is an isometric subgraph of Ξ_n. Let p, q, and P be as in Proposition 2.2. Choose $xy \in E(\Xi_n)$ where $x \in V(M_j)$ and $y \in V(M_j) \cup V(M_{j+1})$. Set $j' := j$ if $y \in V(M_j)$ and $j' := j + 1$ otherwise. Let

$$A = \max\left\{\left\lfloor\frac{j-p}{P}\right\rfloor, 0\right\} \qquad \text{and} \qquad B = \max\left\{\left\lfloor\frac{n-j'-p}{P}\right\rfloor, 0\right\}.$$

Then using Proposition 4.1 we can write

$$\begin{aligned} n(x,y) &= A\cdot\left(n^{(j-q+1)}(x,y) + n^{(j-q+2)}(x,y) + \ldots + n^{(j-p)}(x,y)\right) && (4)\\ &+ \sum_{i=AP+1}^{n-BP} n^{(i)}(x,y) && (5)\\ &+ B\cdot\left(n^{(j'+p)}(x,y) + n^{(j'+p+1)}(x,y) + \ldots + n^{(j'+q-1)}(x,y)\right). && (6)\end{aligned}$$

As p, q and P are defined on the infinite chain graph, it may happen that, for example $n < p$. Also for small and large values of j, the values of A, B, or both can be 0. In these cases the expression remains valid and is even simpler (as some terms vanish).
Each edge of $\Xi_n(M, X)$ is either a copy of an edge from $E(M)$ or a copy of an element from X. Given $u, v \in V(M)$, let $u_i := (u, i)$, $v_i := (v, i)$ $(1 \le i \le n)$ be the corresponding copies of u and v in Ξ_n. The Szeged index $Sz(\Xi_n)$ can be expressed as

$$Sz(\Xi_n) = \sum_{e\in E(M)} Sz_M(\Xi_n, e) + \sum_{e\in X} Sz_X(\Xi_n, e),$$

where $Sz_M(\Xi_n, e)$ and $Sz_X(\Xi_n, e)$ denote the sum of contributions of all copies of e in Ξ_n. More precisely,

$$Sz_M(\Xi_n, e) = \sum_{i=1}^{n} n(u_i, v_i)\cdot n(v_i, u_i), \qquad \text{if } e = uv \in E(M) \tag{7}$$

and

$$Sz_X(\Xi_n, e) = \sum_{i=1}^{n-1} n(u_i, v_{i+1})\cdot n(v_{i+1}, u_i), \qquad \text{if } e = uv \in X. \tag{8}$$

To simplify forthcoming calculations, let us assume that $P = 1$. Then $q = p + 1$. Suppose also that $n \ge 2p - 1$. Take $e = uv \in E(M)$ and let $S^+ = n^{(p)}(u_0, v_0)$, $S^- = n^{(-p)}(u_0, v_0)$,

$$S_i^+ = \sum_{j=0}^{i} n^{(j)}(u_0, v_0), \quad S_i^- = \sum_{j=0}^{i} n^{(-j)}(u_0, v_0) \quad \text{for } 0 \le i \le p-1, \quad \text{and } S_0 = S_0^+ = S_0^-.$$

Then $n(u_i, v_i)$ can be expressed as follows:
If $p \le i \le n + 1 - p$, then

$$n(u_i, v_i) = (i-p)\cdot S^- + (S_{p-1}^- + S_{p-1}^+ - S_0) + (n+1-i-p)\cdot S^+. \tag{9}$$

When $i < p$, we have

$$n(u_i, v_i) = S^-_{i-1} + S^+_{p-1} - S_0 + (n+1-i-p) \cdot S^+ , \qquad (10)$$

and when $i > n+1-p$, we have

$$n(u_i, v_i) = (i-p) \cdot S^- + S^-_{p-1} + S^+_{n+1-i} - S_0 . \qquad (11)$$

Similar expressions also hold for $n(v_i, u_i)$ with appropriately modified values of S^+, S^-, S^+_i, and S^-_i (which we denote by T^+, T^-, T^+_i, and T^-_i, respectively).
Applying (9), (10), and (11) in (7) gives

$$\begin{aligned} Sz_M(\Xi_n, e) &= \sum_{i=1}^{p-1} n(u_i, v_i) \cdot n(v_i, u_i) \\ &+ \sum_{i=p}^{n-p+1} n(u_i, v_i) \cdot n(v_i, u_i) \\ &+ \sum_{i=n-p+2}^{n} n(u_i, v_i) \cdot n(v_i, u_i). \end{aligned} \qquad (12)$$

In more detail, the first summation reads

$$\begin{aligned} \sum_{i=1}^{p-1} n(u_i, v_i) \cdot n(v_i, u_i) &= \sum_{i=1}^{p-1} (S^-_{i-1} + S^+_{p-1} - S_0) \cdot (T^-_{i-1} + T^+_{p-1} - T_0) \\ &+ \sum_{i=1}^{p-1} (n+1-i-p) \cdot S^+ \cdot (T^-_{i-1} + T^+_{p-1} - T_0) \\ &+ \sum_{i=1}^{p-1} (S^-_{i-1} + S^+_{p-1} - S_0) \cdot (n+1-i-p) \cdot T^+ \\ &+ \sum_{i=1}^{p-1} (n+1-i-p) \cdot S^+ \cdot (n+1-i-p) \cdot T^+ \end{aligned}$$

Note that the first term $\sum_{i=1}^{p-1} (S^-_{i-1} + S^+_{p-1} - S_0) \cdot (T^-_{i-1} + T^+_{p-1} - T_0)$ involves a fixed number of arithmetic operations, independent of n. Furthermore, $\sum_{i=1}^{p-1} (n+1-i-p) \cdot S^+ \cdot (T^-_{i-1} + T^+_{p-1} - T_0) = n \sum_{i=1}^{p-1} S^+ \cdot (T^-_{i-1} + T^+_{p-1} - T_0) + \sum_{i=1}^{p-1} (1-i-p) \cdot S^+ \cdot (T^-_{i-1} + T^+_{p-1} - T_0)$ is a linear function in n, and the computation of the coefficients involves a fixed number of operations, independent of n. Similar reasoning applies to the last two terms.
The second summation of (12) gives

$$\begin{aligned} \sum_{i=p}^{n-p+1} n(u_i, v_i) \cdot n(v_i, u_i) &= \sum_{i=p}^{n-p+1} (i-p) \cdot S^- \cdot (i-p) \cdot T^- \\ &+ \sum_{i=p}^{n-p+1} (i-p) \cdot S^- \cdot (T^-_{p-1} + T^+_{p-1} - T_0) \\ &+ \sum_{i=p}^{n-p+1} (i-p) \cdot S^- \cdot (n+1-i-p) \cdot T^+ \\ &+ \sum_{i=p}^{n-p+1} (S^-_{p-1} + S^+_{p-1} - S_0) \cdot (i-p) \cdot T^- \end{aligned}$$

$$
\begin{aligned}
&+ \sum_{i=p}^{n-p+1} (S_{p-1}^{-} + S_{p-1}^{+} - S_0) \cdot (T_{p-1}^{-} + T_{p-1}^{+} - T_0) \\
&+ \sum_{i=p}^{n-p+1} (S_{p-1}^{-} + S_{p-1}^{+} - S_0) \cdot (n+1-i-p) \cdot T^{+} \\
&+ \sum_{i=p}^{n-p+1} (n+1-i-p) \cdot S^{+} \cdot (i-p) \cdot T^{-} \\
&+ \sum_{i=p}^{n-p+1} (n+1-i-p) \cdot S^{+} \cdot (T_{p-1}^{-} + T_{p-1}^{+} - T_0) \\
&+ \sum_{i=p}^{n-p+1} (n+1-i-p) \cdot S^{+} \cdot (n+1-i-p) \cdot T^{+} \\
&= S^{-} \cdot T^{-} \sum_{i=p}^{n-p+1} (i-p)^2 \\
&+ S^{-} \cdot (T_{p-1}^{-} + T_{p-1}^{+} - T_0) \sum_{i=p}^{n-p+1} (i-p) \\
&+ S^{-} \cdot T^{+} \sum_{i=p}^{n-p+1} (i-p) \cdot (n+1-i-p) \\
&+ (S_{p-1}^{-} + S_{p-1}^{+} - S_0) \cdot T^{-} \sum_{i=p}^{n-p+1} (i-p) \\
&+ (S_{p-1}^{-} + S_{p-1}^{+} - S_0) \cdot (T_{p-1}^{-} + T_{p-1}^{+} - T_0)(n-2p+2) \\
&+ (S_{p-1}^{-} + S_{p-1}^{+} - S_0) \cdot T^{+} \sum_{i=p}^{n-p+1} (n+1-i-p) \\
&+ S^{+} \cdot T^{-} \sum_{i=p}^{n-p+1} (n+1-i-p) \cdot (i-p) \\
&+ S^{+} \cdot (T_{p-1}^{-} + T_{p-1}^{+} - T_0) \sum_{i=p}^{n-p+1} (n+1-i-p) \\
&+ S^{+} \cdot T^{+} \sum_{i=p}^{n-p+1} (n+1-i-p)^2 \qquad (13)
\end{aligned}
$$

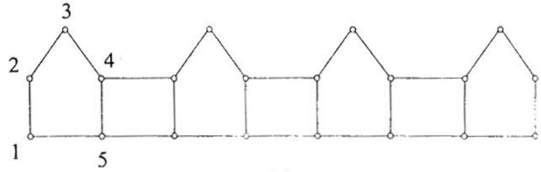
and again, using $\sum_{i=p}^{n-p+1}(n+1-i-p) = \sum_{i=p}^{n-p+1}(i-p) = \frac{1}{2}(n^2+(3-4p)n+(2-6p+4p^2))$, $\sum_{i=p}^{n-p+1}(n+1-i-p)^2 = \sum_{i=p}^{n-p+1}(i-p)^2 = \frac{1}{6}(2n^3+(9-12p)n^2+(13-36p+24p^2)n+(6-26p+36p^2-16p^3))$, and $\sum_{i=p}^{n-p+1}(i-p)(n+1-i-p) = (n-2p)(n-2p+1)(n-2p+2)/6$, one can observe that all terms are polynomial functions of n (of maximal degree 3), and the computation of the coefficients involves a fixed number of arithmetic operations, independent of n.
Similar reasoning applies to the third summation.
Analogous calculation can be performed in the case when $e = uv \in X$.
The above computations are straightforward, but involve a lot of tedious detail. We therefore omit detailed derivation of general formulas. In the next section, complete calculations will be given for several examples.

A natural idea is to let the calculations be carried out by computer, using a programming language which allows symbolic computation. We wrote a *Mathematica*[16] package `SzegedIndex.m` to check calculations in the examples of the next section. The package is given in the Appendix, and is also available, together with an example notebook, at `http://www.fmf.uni-lj.si/~petkovsek/software.html`.
If $P > 1$, it is usually the easiest way to consider each congruence class modulo P separately. Each congruence class can be considered as a special case of the situation when $P = 1$ with appropriately modified values of the preperiod p and S^+, S^-. An example of this approach in presented in Example 2.
We can compute the Szeged index $Sz(\Xi_n(M, X))$ of a fasciagraph $\Xi_n(M, X)$ as a sum of contributions of edges of the monograph and contributions of edges of X. As indicated above, these contributions are polynomial functions of n and the coefficients depend on parameters p, q, P. Furthermore, the computation of coefficients does not depend on n. Hence,

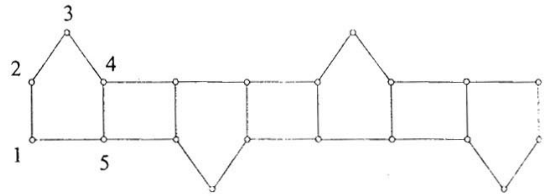
Proposition 4.2 *Closed-form expressions for the Szeged index $Sz(\Xi_n(M, X))$ of a family of fasciagraphs $\Xi_n(M, X)$ $(n \in \mathrm{N})$ can be obtained by an algorithm whose running time depends only on the size of monograph M and does not depend on n.*

5 Examples

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



(a)



(b)

Figure 2: The graphs of Examples 1 and 2.

Example 1. 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 $p = 3$, $q = 4$ and $P = 1$.
Edge contributions to $Sz(\Xi_n(M,X))$ of fasciagraph $\Xi_n(M,X)$ can be computed as follows: For edge $e = (u,v) = (1,5) \in M_0$ the $n^{(i)}(1,5)$ and $n^{(i)}(5,1)$ in the infinite chain graph $\Xi(M,X)$ are

i		-3	-2	-1	0	1	2	3	
$n^{(i)}(1,5)$	...	5	5	5	2	0	0	0	...
$n^{(i)}(5,1)$	...	0	0	0	2	5	5	5	...

The values $n^{(i)}(u,v)$, resp. $n^{(i)}(v,u)$, $(i = 0,1,\ldots)$ can be obtained from matrices D_i by counting the entries of the u-th row that are smaller, resp. larger, than the corresponding entries of the v-th row. The values $n^{(i)}(u,v)$ and $n^{(i)}(v,u)$, $(i = -1,-2\ldots)$ can be obtained from matrices D_i by comparing the respective columns. Another method, which is even simpler for simpler examples, is to read off the values from a picture of the infinite chain graph.
Note that the preperiod for the edge $(1,5)$ is $2 < p$. The contribution of n copies of $e = (1,5) \in M$ to the Szeged index of the fasciagraph $\Xi_n(M,X)$ is hence

$$\begin{aligned} Sz_M(\Xi_n,(1,5)) &= \sum_{j=1}^{n}((j-1)5+2)(2+(n-j)5) = \sum_{j=1}^{n}(4+10(n-1)+25(n-j)(j-1)) \\ &= \sum_{j=1}^{n}(-6-15n+25(n+1)j-25j^2) \\ &= -6n-15n^2+25\frac{n(n+1)^2}{2}-25\frac{n(n+1)(2n+1)}{6} \\ &= \frac{1}{6}n(14-15n+25n^2). \end{aligned} \tag{14}$$

For copies of the edge $e = (1,2) \in M$ we have

i		-3	-2	-1	0	1	2	3	
$n^{(i)}(1,2)$	...	5	3	2	2	3	5	5	...
$n^{(i)}(2,1)$	...	0	0	2	2	0	0	0	...

The contribution of n copies of $e = (1,2)$ is

$$\begin{aligned} Sz_M(\Xi_n,(1,2)) &= 2(2+3+(n-2)5)+4(2+2+3+(n-3)5) \\ &\quad +(n-3)4(3+2+2+3+(n-4)5)+4(2+2+3+(n-3)5) \\ &= 2(23-25n+10n^2). \end{aligned} \quad (15)$$

Note that the expression is valid for $n \geq 4$. For $n = 3$, for example, we have $Sz_M(\Xi_n,(1,2)) = 2(2+3+(n-2)5) + 4(2+2+3+(n-3)5) + (n-3)4(3+2+2+3) + 4(2+2+3 + (n-3)5)$. As we are interested in the asymptotic formulas, we will not compute the expressions for small n explicitly.
By obvious symmetry,

$$Sz_M(\Xi_n,(4,5)) = Sz_M(\Xi_n,(1,2)) = 2(23-25n+10n^2). \quad (16)$$

Similarly, for $e = (2,3)$

i		-3	-2	-1	0	1	2	3	4	
$n^{(i)}(2,3)$	...	5	5	5	2	0	0	0	0	...
$n^{(i)}(3,2)$	...	0	0	0	2	3	2	0	0	...

$$\begin{aligned} Sz_M(\Xi_n,(2,3)) &= \sum_{j=1}^{n-2}(2+5(j-1))(2+3+2)+(2+5(n-2))(2+3)+(2+5(n-1))2 \\ &= \frac{1}{2}(62-77n+35n^2). \end{aligned} \quad (17)$$

and, by symmetry,

$$Sz_M(\Xi_n,(3,4)) = Sz_M(\Xi_n,(2,3)) = \frac{1}{2}(62-77n+35n^2). \quad (18)$$

Now we consider contributions of copies of the two "X-edges". The edge $e = (u,v) = (4,2)$, i.e., the edges $((4,i),(2,i+1))$ $(i = 1,2,\ldots,n-1)$ contribute

i		-3	-2	-1	0	1	2	3	
$n^{(i)}(,)$	...	5	5	5	0	0	0	0	...
$n^{(i)}($,	...	0	0	0	5	5	5	5	...

$$\begin{aligned} Sz_X(\Xi_n,(4,2)) &= \sum_{j=1}^{n-1} 5j5(n-j) \\ &= 25\frac{n^2(n-1)}{2} - 25\frac{(n-1)n(2(n-1)+1)}{6} \\ &= 25\frac{n(n-1)(n+1)}{6}. \end{aligned} \quad (19)$$

Finally, edges of the form $e = (u, v) = ((5, i), (1, i + 1))$ contribute

i		-3	-2	-1	0	1	2	3	
$n^{(i)}(5,1)$	...	5	5	5	0	0	0	0	...
$n^{(i)}(1,5)$	...	0	0	0	5	5	5	5	...

$$Sz_X(\Xi_n, (5,1)) = 25\frac{n(n-1)(n+1)}{6}. \tag{20}$$

Summing all edge contributions we get, for $n \geq 2p - 1 = 5$,

$$Sz(\Xi_n(M,X)) = \frac{1}{2}(308 - 366n + 145n^2 + 25n^3). \tag{21}$$

It may be interesting to compare the results with the value of the Wiener index[11]

$$W = \frac{1}{6}(50n^3 + 105n^2 - 161n + 120). \tag{22}$$

□

Example 2. 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 $p = 2$, $q = 4$, $P = 2$.
Edge contributions to $Sz(\Xi_n(M,X))$ of fasciagraph $\Xi_n(M,X)$ can be computed as follows: For edge $e = (u,v) = (1,5) \in M_0$ the $n^{(i)}(1,5)$ and $n^{(i)}(5,1)$ in the infinite chain graph $\Xi(M,X)$ are

i		-3	-2	-1	0	1	2	3	
$n^{(i)}(1,5)$	...	5	5	5	2	0	0	0	...
$n^{(i)}(5,1)$	...	0	0	0	2	5	5	5	...

The contribution of n copies of edge $e = (1,5) \in M$ to the Szeged index of the fasciagraph $\Xi_n(M,X)$ is hence, as in Example 1,

$$Sz_M(\Xi_n,(1,5)) = \frac{1}{6}n(14-15n+25n^2). \tag{23}$$

For the copies of edge $e=(1,2)\in M$ we have

i		-3	-2	-1	0	1	2	3	
$n^{(i)}(1,2)$	...	0	0	2	2	3	2	3	...
$n^{(i)}(2,1)$	...	2	3	2	2	0	0	0	...

Note that the contribution of the edge (1,5) has period 1 although $P=2$.
The contribution of n copies of edge $e=(1,2)$ have to be considered for n even and n odd separately. For $n=2m$ we get

$$\begin{aligned}
Sz_M(\Xi_n,(1,2)) &= \sum_{j=1}^{2m} n((1,j),(2,j))\cdot n((2,j),(2,1)) = \\
&= \sum_{j=1}^{m}(5j-1)(5(m-j)+4)+\sum_{j=1}^{m-1}(5j+2)(5(m-j)+2)+2\cdot 5m = \\
&= \frac{1}{6}(8+5m)(-3+5m+10m^2),
\end{aligned} \tag{24}$$

and for n odd

$$\begin{aligned}
Sz_M(\Xi_n,(1,2)) &= \sum_{j=1}^{2m+1} n((1,j),(2,j))\cdot n((2,j),(2,1)) = \\
&= \sum_{j=1}^{m}(5j+2)(5(m-j)+4)+\sum_{j=1}^{m}(5j-4)(5(m-j+1)+2)+2(5m+2) = \\
&= \frac{1}{3}(12+83m+90m^2+25m^3).
\end{aligned} \tag{25}$$

By obvious symmetry,

$$Sz_M(\Xi_n,(4,5)) = Sz_M(\Xi_n,(1,2)). \tag{26}$$

Similarly, for $e=(2,3)$

i		-3	-2	-1	0	1	2	3	
$n^{(i)}(2,3)$	...	5	5	5	2	0	0	0	...
$n^{(i)}(3,2)$	...	0	0	0	2	3	5	5	...

$$Sz_M(\Xi_n,(2,3)) = \sum_{j=1}^{n-1}(2+(j-1)5)(2+3+(n-j-1)5)+(2+(n-1)5)2 \tag{27}$$

and since (3,4) is symmetrical to (2,3),

$$Sz_M(\Xi_n,(3,4)) = Sz_M(\Xi_n,(2,3)) = \frac{1}{6}(-36+80n-45n^2+25n^3). \tag{28}$$

Furthermore,

$$Sz_X(\Xi_n,(4,1)) = Sz_X(\Xi_n,(5,2)) = 25\frac{n(n-1)(n+1)}{6} \tag{29}$$

and, summing up all edge contributions, for $n \geq 2p-1 = 3$,

$$Sz(\Xi_n(M,X))) = \begin{cases} \frac{1}{3}(-60+149m-105m^2+550m^3), & n=2m \\ \frac{5}{3}(12+91m+144m^2+110m^3), & n=2m+1 \end{cases} \tag{30}$$

It may be interesting to compare the results with the value of the Wiener index[11]

$$W(\Xi_n(M,X))) = \begin{cases} \frac{1}{24}(-96+134n+75n^2+250n^3), & n \text{ even} \\ \frac{1}{24}(-99+134n+75n^2+250n^3), & n \text{ odd} \end{cases} \tag{31}$$

□

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

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

while the matrices D_2 and D_3 are equal to

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

As $D_3 - D_2 = 2J$, we have $k = 6$, $p = 2$, $q = 3$, $P = 1$, $c = 2$.
The contribution for edge (1,2) can be calculated as follows.

i		-3	-2	-1	0	1	2	3	
$n^{(i)}(1,2)$	...	6	6	6	3	3	6	6	...
$n^{(i)}(2,1)$	...	0	0	0	3	3	0	0	...

$$Sz_M(\Xi_n,(1,2)) = \sum_{j=1}^{n-1}(3+3)(3+3+(n-2)6) + 3(3+(n-1)6) = 9(3-6n+4n^2). \tag{32}$$

It is obvious that

$$Sz_M(\Xi_n,(3,4)) = Sz_M(\Xi_n,(1,2)) = 9(3-6n+4n^2). \tag{33}$$

For edge (2,3) we get

i		-3	-2	-1	0	1	2	3	
$n^{(i)}(2,3)$	...	6	6	6	3	0	0	0	...
$n^{(i)}(3,2)$	...	0	0	0	3	6	6	6	...

$$Sz_M(\Xi_n, (2,3)) = \sum_{j=1}^{n}(3 + 6(j-1))(3 + 6(n-j)) = 3n(1 + 2n^2). \tag{34}$$

Similarly,

$$Sz_M(\Xi_n, (6,5)) = 3n(1 + 2n^2). \tag{35}$$

Finally, for edge (1,6) we get

i		-3	-2	-1	0	1	2	3	
$n^{(i)}(,)$	...	0	0	3	3	0	0	0	...
$n^{(i)}(,)$	...	6	6	3	3	6	6	6	...

By symmetry, the contribution of edge (4,5) is equal to the contribution of edge (1,6), therefore

$$Sz_M(\Xi_n, (1,6)) = Sz_M(\Xi_n, (4,5)) = 9(3 - 6n + 4n^2). \tag{36}$$

For X-edge (4,1) we get

$$Sz_X(\Xi_n, (4,1)) = \sum_{j=1}^{n-1}(6j)(6(n-j)) = 6(n-1)n(n+1) \tag{37}$$

and for X-edge (5,6)

$$Sz_X(\Xi_n, (5,i), (6,i-1)) = 6(n-1)n(n+1). \tag{38}$$

The Szeged index of the fasciagraph of Example 3 is therefore

$$Sz(\Xi_n(M,X)) = 6(18 - 37n + 24n^2 + 4n^3) \qquad \text{for } n \geq 3\,. \tag{39}$$

For comparison, the Wiener index of this family is[11]

$$W(\Xi_n(M,X)) = 12n^3 + 36n^2 - 39n + 18\,. \tag{40}$$

□

Example 4. As our next example, consider again the fasciagraphs obtained by taking 6-cycles C_6 as the monographs and $X = \{(4,6),(3,1)\}$. The matrices $D_0 = D(G)$ and D_1 are

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

while the matrix D_2 is equal to

$$\begin{bmatrix} 6 & 7 & 8 & 9 & 8 & 7 \\ 5 & 6 & 7 & 8 & 7 & 6 \\ 4 & 5 & 6 & 7 & 6 & 5 \\ 5 & 6 & 7 & 6 & 5 & 4 \\ 6 & 7 & 8 & 7 & 6 & 5 \\ 7 & 8 & 9 & 8 & 7 & 6 \end{bmatrix}.$$

As $D_2 - D_1 = 3J$, we have $k = 6$, $p = 1$, $q = 2$, $P = 1$, $c = 3$.
For edge (1,2) we get

i		-3	-2	-1	0	1	2	3	
$n^{(i)}(,)$	...	6	6	6	3	0	0	0	...
$n^{(i)}(,)$	...	0	0	0	3	6	6	6	...

$$Sz_X(\Xi_n, (1,2)) = \sum_{j=1}^{n} (3 + (j-1)6)(3 + (n-j)6) = 3n(1 + 2n^2). \tag{41}$$

By symmetry, the contribution of edge (6,5) is

$$Sz_M(\Xi_n, (6,5)) = Sz_M(\Xi_n, (1,2)) = 3n(1 + 2n^2). \tag{42}$$

and

$$Sz_M(\Xi_n, (2,3)) = Sz_M(\Xi_n, (4,5)) = 3n(1 + 2n^2). \tag{43}$$

For edge (1,6) we get

i		-3	-2	-1	0	1	2	3	
$n^{(i)}(1,6)$	...	3	3	3	3	3	3	3	...
$n^{(i)}(6,1)$	...	3	3	3	3	3	3	3	...

$$Sz_M(\Xi_n, (1,6)) = n \cdot 3n \cdot 3n = 9n^3. \tag{44}$$

By symmetry,

$$Sz_M(\Xi_n, (3,4)) = Sz_M(\Xi_n, (1,6)) = 9n^3. \tag{45}$$

For X-edges (1,3) and (4,6) the contributions are

$$Sz_X(\Xi_n, (1,3)) = Sz_X(\Xi_n, (4,6)) = \sum_{j=1}^{n-1} (6j)(6(n-j)) = 6(n-1)n(n+1). \tag{46}$$

The Szeged index of the fasciagraph of Example 4 is therefore

$$Sz(\Xi_n(M, X)) = 54n^3. \tag{47}$$

□

Example 5. For our last example, consider the monograph obtained from 10-cycle C_{10} by adding the edge connecting two opposite vertices of 10-cycle (vertices 5 and 10) and $X = \{(4,1), (6,9)\}$ (See Figure 3). The matrices $D_0 = D(G)$ and D_1 are

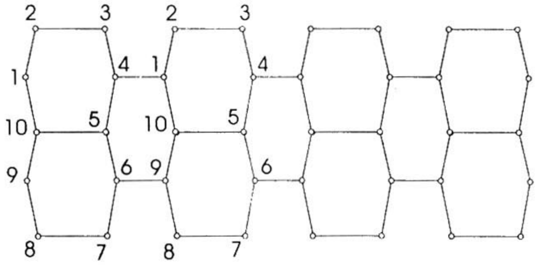


Figure 3: The fasciagraph of example 5 for the case $n = 4$.

$$\begin{bmatrix} 0 & 1 & 2 & 3 & 2 & 3 & 4 & 3 & 2 & 1 \\ 1 & 0 & 1 & 2 & 3 & 4 & 5 & 4 & 3 & 2 \\ 2 & 1 & 0 & 1 & 2 & 3 & 4 & 5 & 4 & 3 \\ 3 & 2 & 1 & 0 & 1 & 2 & 3 & 4 & 3 & 2 \\ 2 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 2 & 1 \\ 3 & 4 & 3 & 2 & 1 & 0 & 1 & 2 & 3 & 2 \\ 4 & 5 & 4 & 3 & 2 & 1 & 0 & 1 & 2 & 3 \\ 3 & 4 & 5 & 4 & 3 & 2 & 1 & 0 & 1 & 2 \\ 2 & 3 & 4 & 3 & 2 & 3 & 2 & 1 & 0 & 1 \\ 1 & 2 & 3 & 2 & 1 & 2 & 3 & 2 & 1 & 0 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 4 & 5 & 6 & 7 & 6 & 7 & 6 & 5 & 4 & 5 \\ 3 & 4 & 5 & 6 & 5 & 6 & 7 & 6 & 5 & 4 \\ 2 & 3 & 4 & 5 & 4 & 5 & 6 & 5 & 4 & 3 \\ 1 & 2 & 3 & 4 & 3 & 4 & 5 & 4 & 3 & 2 \\ 2 & 3 & 4 & 5 & 4 & 5 & 4 & 3 & 2 & 3 \\ 3 & 4 & 5 & 4 & 3 & 4 & 3 & 2 & 1 & 2 \\ 4 & 5 & 6 & 5 & 4 & 5 & 4 & 3 & 2 & 3 \\ 5 & 6 & 7 & 6 & 5 & 6 & 5 & 4 & 3 & 4 \\ 4 & 5 & 6 & 7 & 6 & 7 & 6 & 5 & 4 & 5 \\ 3 & 4 & 5 & 6 & 5 & 6 & 5 & 4 & 3 & 4 \end{bmatrix};$$

while the matrices D_2 and D_3 are equal to

$$\begin{bmatrix} 8 & 9 & 10 & 11 & 10 & 11 & 10 & 9 & 8 & 9 \\ 7 & 8 & 9 & 10 & 9 & 10 & 9 & 8 & 7 & 8 \\ 6 & 7 & 8 & 9 & 8 & 9 & 8 & 7 & 6 & 7 \\ 5 & 6 & 7 & 8 & 7 & 8 & 7 & 6 & 5 & 6 \\ 6 & 7 & 8 & 9 & 8 & 9 & 8 & 7 & 6 & 7 \\ 5 & 6 & 7 & 8 & 7 & 8 & 7 & 6 & 5 & 6 \\ 6 & 7 & 8 & 9 & 8 & 9 & 8 & 7 & 6 & 7 \\ 7 & 8 & 9 & 10 & 9 & 10 & 9 & 8 & 7 & 8 \\ 8 & 9 & 10 & 11 & 10 & 11 & 10 & 9 & 8 & 9 \\ 7 & 8 & 9 & 10 & 9 & 10 & 9 & 8 & 7 & 8 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 12 & 13 & 14 & 15 & 14 & 15 & 14 & 13 & 12 & 13 \\ 11 & 12 & 13 & 14 & 13 & 14 & 13 & 12 & 11 & 12 \\ 10 & 11 & 12 & 13 & 12 & 13 & 12 & 11 & 10 & 11 \\ 9 & 10 & 11 & 12 & 11 & 12 & 11 & 10 & 9 & 10 \\ 10 & 11 & 12 & 13 & 12 & 13 & 12 & 11 & 10 & 11 \\ 9 & 10 & 11 & 12 & 11 & 12 & 11 & 10 & 9 & 10 \\ 10 & 11 & 12 & 13 & 12 & 13 & 12 & 11 & 10 & 11 \\ 11 & 12 & 13 & 14 & 13 & 14 & 13 & 12 & 11 & 12 \\ 12 & 13 & 14 & 15 & 14 & 15 & 14 & 13 & 12 & 13 \\ 11 & 12 & 13 & 14 & 13 & 14 & 13 & 12 & 11 & 12 \end{bmatrix}$$

As $D_2 - D_1 = 4J$, we have $k = 10$, $p = 2$, $q = 3$, $P = 1$, $c = 4$.
For an edge $e \in \{(1,2),(3,4),(4,5),(5,6),(6,7),(8,9),(9,10),(1,10)\}$ we get the same edge contributions to $Sz(\Xi_n(M, X))$:

$$Sz_M(\Xi_n, e) = \frac{1}{3}(-27 + 40n + 50n^3). \tag{48}$$

For edges (2,3), (5,10), and (7,8) we get:

$$Sz_M(\Xi_n,(2,3)) = Sz_M(\Xi_n,(5,10)) = Sz_M(\Xi_n,(7,8)) = \frac{25n}{3}(1 + 2n^2). \tag{49}$$

For X-edges (4,1) and (6,9) we get

$$Sz_X(\Xi_n, (4,1)) = Sz_X(\Xi_n, (6,9)) = \frac{50}{3}(n-1)n(n+1). \tag{50}$$

The Szeged index of the fasciagraph of Example 5 is therefore

$$Sz(\Xi_n(M,X)) = \frac{1}{3}(-216 + 295n + 650n^3) \qquad \text{for } n \geq 3\,. \tag{51}$$

□

Acknowledgement: The authors wish to thank Bojan Mohar for fruitful discussions.

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Appendix: the Mathematica code

```
BeginPackage["SzegedIndex`", "DiscreteMath`Combinatorica`"];

SzegedIndex::usage = "Let G be a graph and X a binary relation on the
vertex set of G. Let F denote the fasciagraph composed of n copies of G
where adjacencies between vertices of two neighbouring copies of G are
determined by X. Then SzegedIndex[G, X, n] gives the Szeged index of F
for large n, provided that each copy of G is an isometric subgraph of F."

Unprotect[Ceiling];
  Ceiling[a_?IntegerQ] := a;
  Ceiling[a_?IntegerQ + b_] := a + Ceiling[b];
  Ceiling[Literal[Times[a__?IntegerQ] + b_.]] := Times[a] + Ceiling[b];
Protect[Ceiling];

Unprotect[Floor];
  Floor[a_?IntegerQ] := a;
  Floor[a_?IntegerQ + b_] := a + Floor[b];
  Floor[Literal[Times[a__?IntegerQ] + b_.]] := Times[a] + Floor[b];
Protect[Floor];

Begin["`Private`"];

TropicalProduct[a_, b_] := Inner[Plus, a, b, Min];

ConstantMatrixQ[a_] := a - a[[1,1]] === 0 * a;

PolySum[t_, {i_, a_Integer, b_Integer}] :=
  Plus @@ Table[t, {i, a, b}];
PolySum[t_, {i_, a_, b_}] /; a =!= 0 :=
  PolySum[Expand[t /. i :> i+a], {i, 0, b-a}];
PolySum[t__Plus, it_] := Expand[PolySum[#, it]& /@ t];
PolySum[c_ t_, {i_, a_, b_}] /; FreeQ[c, i] :=
  Expand[c PolySum[t, {i, a, b}]];
PolySum[c_, {i_, a_, b_}] /; FreeQ[c, i] := Expand[c (b - a + 1)];
PolySum[i_, {i_, 0, n_}] := Expand[n(n + 1)/2];
PolySum[i_^2, {i_, 0, n_}] := Expand[n(n + 1)(2n + 1)/6];
PolySum[i_^m_, {i_, 0, n_}] :=
  Expand[(BernoulliB[m + 1, n + 1] - BernoulliB[m + 1])/(m + 1)];

valPlus[p_, d_, displ_, q_, da_] :=
  Module[{sp, sd, m, mat, mat2, nuP = {}, nvP = {}},
    Do[mat = da[[m]]; mat2 = da[[m + displ]];
       sp = Count[mat2[[p]] - mat[[d]], _?Negative];
       sd = Count[mat2[[p]] - mat[[d]], _?Positive];
       AppendTo[nuP, sp]; AppendTo[nvP, sd], {m, q}];
    Return[{nuP, nvP}]];

valMinus[p_, d_, displ_, q_, da_] :=
  Module[{sp, sd, m, mat, mat2, nuM = {}, nvM = {}},
    Do[mat = Transpose[da[[m]]]; mat2 = Transpose[da[[m + displ]]];
       sp = Count[mat[[p]] - mat2[[d]], _?Negative];
       sd = Count[mat[[p]] - mat2[[d]], _?Positive];
       AppendTo[nuM, sp]; AppendTo[nvM, sd], {m, q}];
    Return[{nuM, nvM}]];

sze[displ_, p_, q_, pp_, da_, m_][e_, remainder_] :=
  Module[{i, j, ee, nuP, nvP, nuM, nvM, a, n = pp * m + remainder},
    {nuP, nvP} = valPlus[e[[1]], e[[2]], displ, q, da];
    {nuM, nvM} = valMinus[e[[1]], e[[2]], displ, q, da];
    i/: IntegerQ[i] = True;
    j/: IntegerQ[j] = True;
    a = Evaluate //@
      (PolySum[ (PolySum[Ceiling[(j-q-i+1)/pp] * nuM[[p+i]], {i, 1, pp}]
        + PolySum[nuM[[i+1]], {i, 0, q-1}]
        + PolySum[nuP[[i+1]], {i, 1, q-1}]
        + PolySum[Ceiling[(n-q-j-i+2)/pp] * nuP[[p+i]], {i, 1, pp}])
      * (PolySum[Ceiling[(j-q-i+1)/pp] * nvM[[p+i]], {i, 1, pp}]
        + PolySum[nvM[[i+1]], {i, 0, q-1}]
        + PolySum[nvP[[i+1]], {i, 1, q-1}]
```

```
      + PolySum[Ceiling[(n-q-j-i+2)/pp] * nvP[[p+i]], {i, 1, pp}]),
         {j, q, n-q+1-displ}]
   + PolySum[ (PolySum[nuM[[i]], {i, 1, j}]
      + PolySum[nuP[[i+1]], {i, 1, q-1}]
      + PolySum[Ceiling[(n-q-j-i+2)/pp] * nuP[[p+i]], {i, 1, pp}])
     * (PolySum[nvM[[i]], {i, 1, j}]
      + PolySum[nvP[[i+1]], {i, 1, q-1}]
      + PolySum[Ceiling[(n-q-j-i+2)/pp] * nvP[[p+i]], {i, 1, pp}]),
         {j, 1, q-1}]
   + PolySum[ (PolySum[Ceiling[(j-q-i+1)/pp] * nuM[[p+i]], {i, 1, pp}]
      + PolySum[nuM[[i+1]], {i, 0, q-1}]
      + PolySum[nuP[[i+1]], {i, 1, n-j}])
     * (PolySum[Ceiling[(j-q-i+1)/pp] * nvM[[p+i]], {i, 1, pp}]
      + PolySum[nvM[[i+1]], {i, 0, q-1}]
      + PolySum[nvP[[i+1]], {i, 1, n-j}]),
         {j, n-q+2-displ, n-displ}]
    /. Ceiling[x_] :> Ceiling[Expand[x]]);
  If[pp > 1,
    ee /: IntegerQ[ee] = True;
    a = a /. Literal[PolySum[x_, {ind_, u_, v_}]] :>
         Plus @@ Table[PolySum[x /. ind :> pp * ee + Mod[r, pp],
           {ee, Ceiling[(u-r)/pp], Floor[(v-r)/pp]}], {r, 0, pp-1}]
      /. {Ceiling[x_] :> Ceiling[Expand[x]],
         Floor[x_] :> Floor[Expand[x]]};
    a = a /. Literal[PolySum[x_, {ind_, u_, v_}]] :>
         PolySum[Expand[x], {ind, u, v}] ];
  Return[a] ];

SzegedIndex[g_Graph, x_List, n_Symbol] :=
 Module[{continue, d, v, t, edges, di, d1, i, j, da, p, q,
        pp, ee, remainder, xx, result, printout, nn},
  Off[Part::pspec];
  nn/: IntegerQ[nn] = True;
  d = AllPairsShortestPath[g]; v = Length[Vertices[g]];
  t = ReplacePart[Table[Infinity, {i, v}, {j, v}], 1, x];
  edges = ToUnorderedPairs[g]; di = TropicalProduct[d, t];
  d1 = TropicalProduct[di, d]; di = d1; i = 1; da = {d1};
  continue = True;
  While[continue,
    di = TropicalProduct[di, d1]; AppendTo[da, di];
    While[i > 0 && continue,
      If[ConstantMatrixQ[di - da[[i]]],
        continue = False; p = i; q = Length[da],
         i--] ];
    If[continue, i = Length[da]] ];
  da = Prepend[da, d]; pp = q - p;
  Do[ee = {edges, Table[remainder, {Length[edges]}]};
    xx = {x, Table[remainder, {Length[x]}]};
    result = Factor[
      Plus @@ MapThread[sze[0, p, q, pp, da, nn], ee] +
      Plus @@ MapThread[sze[1, p, q, pp, da, nn], xx]] /. nn -> n;
    If[pp > 1,
       printout = {n >= Ceiling[(2p - 1 - remainder) / pp],
                  ":   Sz(", pp * n};
       If[remainder > 0,
          printout = Join[printout, {"+", remainder}] ];
       printout = Join[printout, {") = ", result}],
         printout = {n >= 2p - 1, ":   Sz(n) = ", result}];
    Print @@ printout,
   {remainder, 0, pp - 1}];
   On[Part::pspec] ];

End[ ];

EndPackage[ ];
```