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A New Alternative to Szeged, Mostar, and PI Polynomials—The SMP Polynomials

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Abstract: Szeged-like topological indices are well-studied distance-based molecular descriptors, which include, for example, the (edge-)Szeged index, the (edge-)Mostar index, and the (vertex-)PI index. For these indices, the corresponding polynomials were also defined, i.e., the (edge-)Szeged polynomial, the Mostar polynomial, the PI polynomial, etc. It is well known that, by evaluating the first derivative of such a polynomial at $x = 1$, we obtain the related topological index. The aim of this paper is to introduce and investigate a new graph polynomial of two variables, which is called the SMP polynomial, such that all three vertex versions of the above-mentioned indices can be easily calculated using this polynomial. Moreover, we also define the edge-SMP polynomial, which is the edge version of the SMP polynomial. Various properties of the new polynomials are studied on some basic families of graphs, extremal problems are considered, and several open problems are stated. Then, we focus on the Cartesian product, and we show how the (edge-)SMP polynomial of the Cartesian product of n graphs can be calculated using the (weighted) SMP polynomials of its factors.

Keywords: SMP polynomial; edge-SMP polynomial; Cartesian product; Szeged index; Mostar index; PI index

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1. Introduction and Preliminaries

Distance-based topological indices are extensively used in mathematical chemistry in order to predict physico-chemical properties of chemical compounds from the underlying molecular graph. One of the most important distance-based molecular descriptors is the well-known Wiener index [1], which is defined as the sum of distances between all pairs of vertices in a given graph. More precisely, for a connected graph G, the *Wiener index* $W(G)$ is calculated as

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u,v),$$

where $d_G(u,v)$ denotes the usual shortest path distance between vertices u and v of G. See [2] for a recent review on the Wiener index.

It is easy to see that, if T is a tree, then the Wiener index can be computed as

$$W(T) = \sum_{e=uv \in E(T)} n_u(e|T) n_v(e|T), \tag{1}$$

where $n_u(e|T)$ denotes the number of vertices of T whose distance to u is smaller than the distance to v and $n_v(e|T)$ is defined analogously. Therefore, in 1994, Gutman used the right-hand side of (1) to define the so-called Szeged index for any connected graph G [3], which turned out to be useful in various applications. As a consequence, many different variations and also edge versions of this index were considered—for example, the PI index [4], the vertex-PI index [5], the edge-Szeged index [6], the Mostar index [7], and the edge-Mostar index [8]. In particular, the Mostar index recently attracted quite a lot of attention, since it can be used as a measure of peripherality in molecular graphs and networks [9]. Note that all these indices belong to the family of Szeged-like topological indices [10].

In order to formally introduce Szeged-like topological indices, we need additional notation. Let G be a connected graph. The distance between a vertex x and an edge $e = uv$ is defined as $d_G(x,e) = \min\{d_G(x,u), d_G(x,v)\}$. In addition, if $e = uv$ is any edge of G, then the following notation for the sets of vertices and edges of G will be used:

$$\begin{aligned}
N_u(e|G) &= \{x \in V(G) \mid d_G(x,u) < d_G(x,v)\},\\
N_v(e|G) &= \{x \in V(G) \mid d_G(x,v) < d_G(x,u)\},\\
N_0(e|G) &= \{x \in V(G) \mid d_G(x,u) = d_G(x,v)\},\\
M_u(e|G) &= \{f \in E(G) \mid d_G(u,f) < d_G(v,f)\},\\
M_v(e|G) &= \{f \in E(G) \mid d_G(v,f) < d_G(u,f)\},\\
M_0(e|G) &= \{f \in E(G) \mid d_G(u,f) = d_G(v,f)\}.
\end{aligned}$$

Moreover, let

$$\begin{array}{lll}
n_u(e|G) = |N_u(e|G)|, & n_v(e|G) = |N_v(e|G)|, & n_0(e|G) = |N_0(e|G)|,\\
m_u(e|G) = |M_u(e|G)|, & m_v(e|G) = |M_v(e|G)|, & m_0(e|G) = |M_0(e|G)|.
\end{array}$$

Obviously, $n_u(e|G)$ represents the number of vertices of G that are closer to u than to v and $m_u(e|G)$ is the number of edges of G that are closer to u than to v.

For a connected graph G with at least one edge, we can now define the *Szeged index* $Sz(G)$, the *Mostar index* $Mo(G)$, and the *vertex-PI index* $PI_v(G)$ in the following way:

$$\begin{aligned}
Sz(G) &= \sum_{e=uv\in E(G)} n_u(e|G)n_v(e|G),\\
Mo(G) &= \sum_{e=uv\in E(G)} |n_u(e|G) - n_v(e|G)|,\\
PI_v(G) &= \sum_{e=uv\in E(G)} (n_u(e|G) + n_v(e|G)).
\end{aligned}$$

The edge versions of these indices are defined analogously. Below is the *edge-Szeged index* $Sz_e(G)$, the *edge-Mostar index* $Mo_e(G)$, and the *PI index* $PI(G)$:

$$\begin{aligned}
Sz_e(G) &= \sum_{e=uv\in E(G)} m_u(e|G)m_v(e|G),\\
Mo_e(G) &= \sum_{e=uv\in E(G)} |m_u(e|G) - m_v(e|G)|,\\
PI(G) &= \sum_{e=uv\in E(G)} (m_u(e|G) + m_v(e|G)).
\end{aligned}$$

In some cases, it is useful to consider graph polynomials related to distance-based topological indices, since such polynomials provide much more information about the topology of a given graph. The most investigated among these polynomials is the Hosoya polynomial (also called Wiener polynomial), which is closely related to the Wiener index and was introduced in 1988 by Hosoya [11]. It is well known that the Wiener index of a graph G can be computed by evaluating the first derivative of the Hosoya polynomial at $x = 1$.

Similarly, graph polynomials related to Szeged-like topological indices can also be introduced—for example, the *Szeged polynomial* $Sz(G;x)$ [12], the *edge-Szeged polynomial* $Sz_e(G;x)$ [13], the *Mostar polynomial* $Mo(G;x)$ [9], the *edge-Mostar polynomial* $Mo_e(G;x)$, the *vertex-PI polynomial* $PI_v(G;x)$ [14], and the *PI polynomial* $PI(G;x)$ [15]. For a connected graph G, these polynomials are defined with the following formulas:

$$Sz(G;x) = \sum_{e=uv\in E(G)} x^{n_u(e|G)n_v(e|G)}, \qquad Sz_e(G;x) = \sum_{e=uv\in E(G)} x^{m_u(e|G)m_v(e|G)},$$
$$Mo(G;x) = \sum_{e=uv\in E(G)} x^{|n_u(e|G)-n_v(e|G)|}, \qquad Mo_e(G;x) = \sum_{e=uv\in E(G)} x^{|m_u(e|G)-m_v(e|G)|},$$
$$PI_v(G;x) = \sum_{e=uv\in E(G)} x^{n_u(e|G)+n_v(e|G)}, \qquad PI(G;x) = \sum_{e=uv\in E(G)} x^{m_u(e|G)+m_v(e|G)}.$$

Additional investigations on these graph polynomials can be found, for example, in [16–22]. Recently, several so-called root-indices of graphs were defined by using Szeged-like polynomials [23]. It is interesting that the mentioned root-indices have a higher ability to discriminate graphs than the corresponding standard indices.

Let $TI \in \{Sz, Sz_e, Mo, Mo_e, PI_v, PI\}$ be a topological index and P the corresponding graph polynomial. It is obvious that, for any connected graph G, the topological index $TI(G)$ can be calculated as the first derivative of the polynomial P at $x = 1$, i.e.,

$$TI(G) = P'(G;1).$$

The aim of this paper is to define such a graph polynomial that the Szeged index, the Mostar index, and the vertex-PI index can all be calculated by using only this one polynomial. It turns out that the mentioned goal can be achieved by introducing a polynomial of two variables, which we call the SMP polynomial. Similarly, one can also define the edge-SMP polynomial, which can be used to compute the edge-Szeged index, the edge-Mostar index, and the PI index.

The structure of the paper is the following: in the next section, we formally introduce the SMP polynomial, the edge-SMP polynomial, and also the weighted version of these polynomials. In Section 3, we investigate some basic properties of the (edge-)SMP polynomial. In particular, we focus on some basic families of graphs, trees, and extremal problems related to SMP polynomials. Moreover, several open problems are stated. Finally, in Section 4, we consider Cartesian products of graphs and provide formulas for calculating the (edge-)SMP polynomial of the Cartesian product $G = G_1\square G_2\square \cdots \square G_n$ by using the (weighted) SMP polynomials of its factors. Note that some existing results related to Szeged-like topological indices and polynomials of Cartesian products can be found in [5,12,18,24,25].

2. The SMP Polynomials

As already mentioned, we introduce a new graph polynomial of two variables, which can be used to easily compute the Szeged index, the Mostar index, and the vertex-PI index of a given graph.

In the rest of the paper, we always assume that G is a connected graph with at least one edge, although sometimes this is not specifically mentioned.

Definition 1. *Let G be a connected graph with at least one edge. The **SMP polynomial** of G, denoted as $SMP(G;x,y)$, is defined as*

$$SMP(G;x,y) = \sum_{\substack{e=uv\in E(G),\\ n_u(e)\geq n_v(e)}} x^{n_u(e|G)} y^{n_v(e|G)}.$$

The next proposition is obvious, and it shows how partial derivatives of the SMP polynomial can be applied to calculate the above-mentioned topological indices.

Proposition 1. *If G is a connected graph, then*

$$\begin{aligned} Sz(G) &= \left(\frac{\partial}{\partial x}\left(\frac{\partial}{\partial y} SMP(G;x,y)\right)\right)\Big|_{x=y=1}, \\ Mo(G) &= \left(\frac{\partial}{\partial x} SMP\left(G;x,\frac{1}{x}\right)\right)\Big|_{x=1}, \\ PI_v(G) &= \left(\frac{\partial}{\partial x} SMP(G;x,x)\right)\Big|_{x=1}. \end{aligned}$$

Note that the advantage of the introduced polynomial is the fact that one has to consider only one polynomial instead of three to compute three well-known molecular descriptors. In addition, by combining different operations, several other topological indices can be defined and computed from the same polynomial.

Similarly, we can introduce the edge version of the SMP polynomial, which is closely related to the edge-Szeged index, the edge-Mostar index, and the PI index.

Definition 2. *Let G be a connected graph with at least one edge. The* ***edge-SMP polynomial*** *of G, denoted as $SMP_e(G;x,y)$, is defined as*

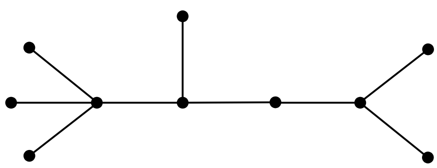
$$SMP(G;x,y) = \sum_{\substack{e=uv\in E(G),\\ m_u(e)\geq m_v(e)}} x^{m_u(e|G)} y^{m_v(e|G)}.$$

The following proposition can be stated.

Proposition 2. *If G is a connected graph, then*

$$\begin{aligned} Sz_e(G) &= \left(\frac{\partial}{\partial x}\left(\frac{\partial}{\partial y} SMP_e(G;x,y)\right)\right)\Big|_{x=y=1}, \\ Mo_e(G) &= \left(\frac{\partial}{\partial x} SMP_e\left(G;x,\frac{1}{x}\right)\right)\Big|_{x=1}, \\ PI(G) &= \left(\frac{\partial}{\partial x} SMP_e(G;x,x)\right)\Big|_{x=1}. \end{aligned}$$

To show an example, let T be a tree from Figure 1.



T

Figure 1. Tree T.

Obviously, T contains six different edges $e = uv$ for which $\{n_u(e|T), n_v(e|T)\} = \{9,1\}$ and $\{m_u(e|T), m_v(e|T)\} = \{8,0\}$. Moreover, there are two edges $e = uv$ for which $\{n_u(e|T), n_v(e|T)\} = \{6,4\}$ and $\{m_u(e|T), m_v(e|T)\} = \{5,3\}$. In addition, for one edge, it holds $\{n_u(e|T), n_v(e|T)\} = \{7,3\}$ and $\{m_u(e|T), m_v(e|T)\} = \{6,2\}$. Therefore, the corresponding SMP polynomials are:

$$\begin{aligned} SMP(T;x,y) &= 6x^9y + x^7y^3 + 2x^6y^4, \\ SMP_e(T;x,y) &= 6x^8 + x^6y^2 + 2x^5y^3. \end{aligned}$$

It is useful to also define the weighted SMP polynomial of a graph with two weights on the edges, which will be needed in Section 4. Therefore, let G be a graph and let $w_1, w_2 : E(G) \to [0, \infty)$ be two weights on the edges of G. The triple (G, w_1, w_2) is then called a *double edge-weighted graph*.

Definition 3. *Let (G, w_1, w_2) be a double edge-weighted connected graph with at least one edge. The **weighted SMP polynomial** of (G, w_1, w_2), denoted as $SMP_{(w_1,w_2)}(G;x,y)$, is defined in the following way:*

$$SMP_{(w_1,w_2)}(G;x,y) = \sum_{e \in E(G)} x^{w_1(e)} y^{w_2(e)}. \tag{2}$$

Obviously, the SMP polynomial and the edge-SMP polynomial are just special cases of the weighted SMP polynomial. More precisely, if for any edge $e = uv \in E(G)$, we define

$$n_1(e) = \max\{n_u(e|G), n_v(e|G)\}, \quad n_2(e) = \min\{n_u(e|G), n_v(e|G)\}$$

and

$$m_1(e) = \max\{m_u(e|G), m_v(e|G)\}, \quad m_2(e) = \min\{m_u(e|G), m_v(e|G)\},$$

then it holds

$$SMP(G;x,y) = SMP_{(n_1,n_2)}(G;x,y) \text{ and } SMP_e(G;x,y) = SMP_{(m_1,m_2)}(G;x,y).$$

3. Basic Properties of SMP Polynomials

In this section, several properties of SMP polynomials are discussed. We start with the following observation related to bipartite graphs.

Proposition 3. *Let G be a connected graph on n vertices, where $n \geq 2$. Then, G is bipartite if and only if, in every term $a_{i,j}x^iy^j$ of $SMP(G;x,y)$, we have $i + j = n$.*

Proof. Let $e = uv$ be an edge of G. If G is bipartite, then, for every vertex w, we have $d_G(u,w) \neq d_G(v,w)$, which means that $n_u(e|G) + n_v(e|G) = n$.

On the other hand, if G is non-bipartite, let C be a shortest odd cycle in G. Observe that, if $u, v \in V(C)$, then $d_G(u,v) = d_C(u,v)$; otherwise, G has an odd cycle which is shorter than C. Let $e = u_1u_2$ be an edge in C and let w be a vertex on C opposite to e. Then, $d_C(u,w) = d_C(v,w)$ and consequently $d_G(u,w) = d_G(v,w)$, which means that $n_u(e|G) + n_v(e|G) \leq n - 1$. □

Now, we focus on trees and firstly provide the relation between the SMP polynomial and the edge-SMP polynomial in this class of graphs.

Proposition 4. *If T is a tree, then $SMP_e(T;x,y) = \frac{1}{xy}SMP(T;x,y)$.*

Proof. Let $e = uv$ be an edge of T. For every other edge $e' = u'v'$, denote by $w_{e'}$ that vertex from u' and v', which has a bigger distance from e. Since T is a tree, $w_{e'}$ is defined uniquely. Then, $N_u(e|T)$ contains the vertices $\{w_{e'} \mid e' \in M_u(e|T)\} \cup \{u\}$ and $N_v(e|T)$ contains the vertices $\{w_{e'} \mid e' \in M_v(e|T)\} \cup \{v\}$. Therefore, $n_u(e|T) = m_u(e|T) + 1$ and $n_v(e|T) = m_v(e|T) + 1$, and consequently $SMP_e(T;x,y) = \frac{1}{xy}SMP(T;x,y)$. □

Hence, for trees, it suffices to consider $SMP(T;x,y)$.

By definition, $SMP(G;1,1)$ equals the number of edges in G. Since the only connected graphs with n vertices and $n-1$ edges are trees, we have the following observation.

Observation 1. *Let G be a connected graph on n vertices. Then, G is a tree if and only if $SMP(G;1,1) = n-1$.*

Next, some special families of trees are considered. As usual, by P_n and S_n, we denote a path and a star, respectively, on n vertices. Take an edge e. Attach a pendant edges to one endvertex of e and attach b pendant vertices to the other endvertex of e, where $a \geq b$. The resulting graph is called a double star, and it is denoted by $D_{a,b}$. Observe that $D_{a,b}$ has $a+b+2$ vertices. We have

$$SMP(P_n, x, y) = \begin{cases} 2\sum_{i=1}^{n/2-1} x^{n-i}y^i + x^{n/2}y^{n/2} \text{ if } n \text{ is even,} \\ 2\sum_{i=1}^{(n-1)/2} x^{n-i}y^i \text{ if } n \text{ is odd;} \end{cases}$$
$$SMP(S_n, x, y) = (n-1)x^{n-1}y;$$
$$SMP(D_{a,b}, x, y) = (a+b)x^{a+b+1}y + x^{a+1}y^{b+1}.$$

We can prove the next statement related to the uniqueness of the SMP polynomial.

Proposition 5. *Let $T \in \{P_n, S_n, D_{a,b}\}$ and let $P(x,y) = SMP(T;x,y)$. Then, the unique connected graph with polynomial $P(x,y)$ is T.*

Proof. Let $SMP(G;x,y) = P(x,y)$. Then, G has $m = P(1,1)$ edges. Consider one term of $P(x,y)$, say $a_{i,j}x^iy^j$. Then, G contains an edge (in fact, it contains at least $a_{i,j}$ edges), which is in a component with at least $i+j$ vertices. By Proposition 3 and Observation 1, $i+j = m+1$. Hence, all edges are in a single component, and G is a tree.

Denote $n = m+1$. If $e = uv$ is a pendant edge of a tree, then $\{n_u(e|G), n_v(e|G)\} = \{n-1, 1\}$, and if e is not pendant, then $\{n_u(e|G), n_v(e|G)\} = \{i,j\}$, where $2 \leq i,j \leq n-2$. Hence, $P(x,y)$ contains a term $qx^{n-1}y$, and q is the number of pendant edges in G. Consequently, G has q pendant vertices, which solve the cases $T \in \{P_n, S_n\}$.

In the last case, $q = n-2$. Hence, the tree G contains $n-2$ pendant edges and one edge, say f, which is not pendant. Let x^iy^j be the term of $P(x,y)$ for which $2 \leq i,j \leq n-2$. Then, to one endvertex of e, there are attached $i-1$ pendant vertices and, to the other endvertex of e, there are attached $j-1$ pendant vertices. Thus, T is $D_{i-1,j-1}$. □

It is also interesting to investigate trees with the same SMP polynomials. One can check that the smallest nonisomorphic trees T_1 and T_2, for which $SMP(T_1;x,y) = SMP(T_2;x,y)$, have seven vertices and four pendant edges; see Figure 2. More precisely, $SMP(T_1;x,y) = SMP(T_2;x,y) = 4x^6y + x^5y^2 + x^4y^3$. Note also that there exist 11 nonisomorphic trees on seven vertices, but only T_1 and T_2 have the same SMP polynomials.

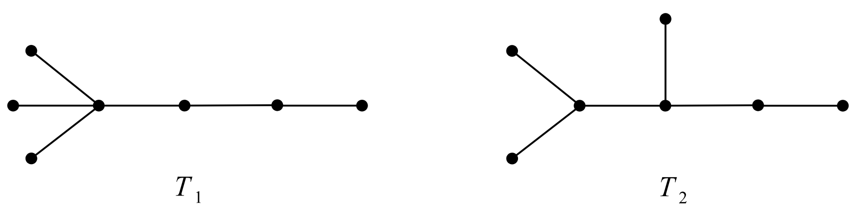


Figure 2. Trees T_1 and T_2 with equal SMP polynomials.

Now, we consider graphs which are not trees. By C_n, K_n and K_{n_1,n_2}, we denote a cycle, a complete graph and a complete bipartite graph, respectively, on n vertices. In the last case, $n = n_1 + n_2$, and we also assume $n_1 \geq n_2$. We have

$$SMP(C_n;x,y) = nx^{n/2}y^{n/2} \text{ and } SMP_e(C_n;x,y) = nx^{(n-2)/2}y^{(n-2)/2} \text{ if } n \text{ is even;}$$
$$SMP(C_n;x,y) = nx^{(n-1)/2}y^{(n-1)/2} \text{ and } SMP_e(C_n;x,y) = nx^{(n-1)/2}y^{(n-1)/2} \text{ if } n \text{ is odd;}$$
$$SMP(K_n;x,y) = \tbinom{n}{2}xy \text{ and } SMP_e(K_n;x,y) = \tbinom{n}{2}x^{n-2}y^{n-2};$$
$$SMP(K_{n_1,n_2};x,y) = n_1n_2x^{n_1}y^{n_2} \text{ and } SMP_e(K_{n_1,n_2};x,y) = n_1n_2x^{n_1-1}y^{n_2-1}.$$

The case of odd cycles opens the following:

Problem 1. *Characterize graphs G, for which $SMP(G;x,y) = SMP_e(G;x,y)$.*

If a graph G is edge-transitive on m edges, then there are i_1, j_1 and i_2, j_2, such that $SMP(G;x,y) = mx^{i_1}y^{j_1}$ and $SMP_e(G;x,y) = mx^{i_2}y^{j_2}$. For example, let O_3 be the Petersen graph and let Q_t be the graph of t-dimensional cube. Observe that Q_t has 2^t vertices and $t2^{t-1}$ edges. We have

$$SMP(O_3;x,y) = 15x^2y^2 \text{ and } SMP_e(O_3;x,y) = 15x^6y^6;$$
$$SMP(Q_t;x,y) = t2^{t-1}x^{2^{t-1}}y^{2^{t-1}} \text{ and } SMP_e(Q_t;x,y) = t2^{t-1}x^{(t-1)2^{t-2}}y^{(t-1)2^{t-2}}.$$

If G is edge-transitive, then there are integers i and j (not necessarily positive), such that $SMP_e(G;x,y)/SMP(G;x,y) = x^iy^j$. Denote $\varphi(G) = i + j$.

Observe that $\varphi(K_n) = 2n - 6$ and $\varphi(K_{n_1,n_2}) = -2$, while, for even n, we also have $\varphi(C_n) = -2$. Moreover, $\varphi(O_3) = 8$ and $\varphi(Q_t) = 2^{t-1}(t-3)$. It would be interesting to find extremal values of φ. Therefore, we state the following problem:

Problem 2. *Characterize edge-transitive graphs on n vertices with an extremal value of φ.*

Moreover, what are the graphs with the second or third extremal value of φ?

Next, we consider bounds for the degree of SMP and SMP_e. We set

$$n(G) = \max\{n_u(e|G) + n_v(e|G) \mid e = uv \in E(G)\},$$
$$m(G) = \max\{m_u(e|G) + m_v(e|G) \mid e = uv \in E(G)\}.$$

Observe that $n(G)$ is the degree of $SMP(G;x,y)$, and $m(G)$ is the degree of $SMP_e(G;x,y)$. In the next statement, we bound the degree of $SMP(G;x,y)$.

Proposition 6. *Let G be a connected graph on n vertices, where $n \geq 2$.*

- *If $n(G)$ is maximum possible, then $n(G) = n$, and extremal graphs include all bipartite graphs and graphs having a bridge.*
- *If $n(G)$ is minimum possible, then $n(G) = 2$, and G is the complete graph K_n.*

Proof. First, we consider the upper bound. For every edge $e = uv$, we have $n_u(e|G) + n_v(e|G) \leq n$, which means that $n(G) \leq n$. By Proposition 3, if $e = uv$ is an edge of a bipartite graph, then $n_u(e|G) + n_v(e|G) = n$ and so $n(G) = n$ if G is bipartite. The same is true if e is a bridge, and so, if G is a graph with a bridge, then $n(G) = n$ as well.

Now, we consider the lower bound. For every edge $e = uv$, we have $n_u(e|G) \geq 1$ since $0 = d(u,u) < d(v,u) = 1$. By symmetry, also $n_v(e|G) \geq 1$, and so $n_u(e|G) + n_v(e|G) \geq 2$. If $n_u(e|G) + n_v(e|G) = 2$, then every neighbour of u (other then v) must be a neighbour of v, and every neighbour of v (other than u) must be a neighbour of u. Consequently, if $n(G) = 2$, then every pair x, y of adjacent vertices must have the same neighbours in $V(G) \setminus \{x,y\}$. Hence, G is the complete graph K_n. □

Take a complete graph on $n-1$ vertices K_{n-1}, attach a pendant vertex to one of the vertices of K_{n-1}, and denote the resulting graph by K_{n-1}^{+}. In the following theorem, we give a tight upper bound for the degree of $SMP_e(G;x,y)$.

Theorem 1. *Let G be a connected graph on n vertices, $n \geq 2$, for which $m(G)$ is maximum possible. Then, $m(G) = \binom{n-1}{2}$ if $n \geq 5$ and $m(G) = 2n-4$ if $n \leq 5$. Moreover, if $n \geq 6$, then K_{n-1}^{+} is the unique extremal graph.*

Proof. Let $e = uv$ be an edge, such that $m_u(e|G) + m_v(e|G) = m(G)$. If $\deg(u) = \deg(v) = n-1$, then every edge which is not adjacent to e has distance 1 from both u and v. Hence, $m(G) = 2n-4$ since $d(u,e) = d(v,e)$.

In the following, we may assume that $n > 2$ and $\deg(v) < n-1$. Thus, there is a vertex, say w, which is not adjacent to v. Let x be a vertex of $V(G) \setminus \{u,v,w\}$. We consider possible edges ux, vx and wx. If $ux, vx \in E(G)$, then $d(u,wx) = d(v,wx) = 1$, so at most two edges from $\{ux,vx,wx\}$ contribute to $m_u(e|G) + m_v(e|G)$. Since for $x,y \in V(G) \setminus \{u,v,w\}$, where $x \neq y$, the sets $\{ux,vx,wx\}$ and $\{uy,vy,wy\}$ are disjoint, e does not contribute to $m_u(e|G) + m_v(e|G)$, and $vw \notin E(G)$, we have

$$m(G) \leq \binom{n}{2} - (n-3) - 1 - 1 = \binom{n-1}{2}.$$

However, if $e' = u'v'$ is the pendant edge of K_{n-1}^{+}, then $m_{u'}(e'|K_{n-1}^{+}) + m_{v'}(e'|K_{n-1}^{+}) = \binom{n-1}{2}$. Since $\binom{n-1}{2} > 2n-4$ if $n \geq 6$ (observe that equality holds if $n = 5$), we have $m(G) = \binom{n-1}{2}$ if $n \geq 6$ and $m(G) = 2n-4$, otherwise.

Now assume that $n \geq 6$ and G is an extremal graph. As explained above, $m(G)$ is attained on $e = uv$ for which $\deg(v) < n-1$. Thus, there is $w \in V(G)$ such that $vw \notin E(G)$. Moreover, G contains all edges which have both endvertices in $V(G) \setminus \{u,v,w\}$ and also uw.

Suppose that there is $x \in V(G) \setminus \{u,v,w\}$, such that $vx \in E(G)$. Since $n \geq 6$, there is a vertex $y \in V(G) \setminus \{u,v,w,x\}$. As mentioned above, $xy \in E(G)$ and xy contributes to $m_u(e|G) + m_v(e|G)$. Since $d(v,xy) = 1$, we have $ux \notin E(G)$. However, two edges from the triple $\{ux,vx,wx\}$ must contribute to $m_u(e|G) + m_v(e|G)$, and so $wx \in E(G)$. Since $uw, vx \in E(G)$, we have $d(u,wx) = d(v,wx)$ and so wx cannot contribute to $m_u(e) + m_v(e)$, a contradiction. Hence, $vx \notin E(G)$ for $x \neq u$ and consequently G is K_{n-1}^{+}. $\square$

Since we do not know a tight lower bound for the degree of $SMP_e(G;x,y)$, we have the following problem.

Problem 3. *Find a tight lower bound for $m(G)$ and characterize the extremal graphs.*

In some chemical applications, it is interesting to consider a polynomial of (molecular) graphs for particular values of x any y, since in this way it is possible to obtain a molecular descriptor from the polynomial. For an example, see [26]. Therefore, we finish this section with the next open problem.

Problem 4. *Characterize graphs with extremal value of $SMP(G;c_1,c_2)$ or $SMP_e(G;c_1,c_2)$ for a given pair (c_1,c_2).*

4. SMP Polynomials of Cartesian Products

In this section, we investigate the SMP polynomial and the edge-SMP polynomial of Cartesian products of graphs. First, we present some basic definitions from [27].

The *Cartesian product* of graphs $G_1, G_2, \ldots, G_n$ is the graph $G = G_1 \square G_2 \square \cdots \square G_n$ such that:

- $V(G) = V(G_1) \times V(G_2) \times \cdots \times V(G_n)$,

- two vertices $a = (a_1, a_2, \ldots, a_n)$, $b = (b_1, b_2, \ldots, b_n) \in V(G)$ are adjacent in G if and only if there exists exactly one $k \in \{1, \ldots, n\}$ such that $a_k b_k \in E(G_k)$ and $a_i = b_i$ for every $i \in \{1, \ldots, n\} \setminus \{k\}$.

For a vertex x of the Cartesian product G, the k-th coordinate of x will be denoted as x_k for any $k \in \{1, \ldots, n\}$, i.e., $x = (x_1, x_2, \ldots, x_n)$.

In addition, for the Cartesian product $G = G_1 \Box G_2 \Box \cdots \Box G_n$ and $k \in \{1, \ldots, n\}$, we use the following notation:

$$E_k(G) = \{uv \in E(G) \mid u_k v_k \in E(G_k)\}.$$

Observe that the sets $E_1(G), E_2(G), \ldots, E_n(G)$ are pairwise disjoint and

$$E(G) = E_1(G) \cup E_2(G) \cup \cdots \cup E_n(G). \tag{3}$$

It is well known that the Cartesian product G is connected if and only if all the factors G_k, $k \in \{1, \ldots, n\}$, are connected. Moreover, for vertices $a, b \in V(G)$, the following distance formula holds true [27]:

$$d_G(a, b) = \sum_{k=1}^{n} d_{G_k}(a_k, b_k). \tag{4}$$

We denote $r = |V(G)|$ and $s = |E(G)|$, where $G = G_1 \Box G_2 \Box \cdots \Box G_n$ is the Cartesian product. In addition, let $r_k = |V(G_k)|$ and $s_k = |E(G_k)|$ for any $k \in \{1, \ldots, n\}$. Obviously, we have

$$r = |V(G)| = \prod_{k=1}^{n} |V(G_k)| = r_1 r_2 \cdots r_n. \tag{5}$$

In addition, since

$$|E_k(G)| = |E(G_k)| \cdot \prod_{\substack{i=1 \\ i \neq k}}^{n} |V(G_i)| = s_k \frac{r}{r_k},$$

from Equation (3) one can obtain

$$s = |E(G)| = \sum_{k=1}^{n} |E_k(G)| = r \sum_{k=1}^{n} \frac{s_k}{r_k}. \tag{6}$$

Moreover, for $k \in \{1, \ldots, n\}$, we use the following notation:

$$G/G_k = G_1 \Box \cdots \Box G_{k-1} \Box G_{k+1} \Box \cdots \Box G_n.$$

As a consequence, by using Equations (5) and (6), we also have

$$|V(G/G_k)| = \frac{r}{r_k} \quad \text{and} \quad |E(G/G_k)| = \frac{r}{r_k} \sum_{\substack{i=1 \\ i \neq k}}^{n} \frac{s_i}{r_i}. \tag{7}$$

Next, we investigate some subsets of vertices in Cartesian products of graphs in order to calculate the SMP polynomial.

Proposition 7. *Suppose that $G = G_1 \square G_2 \square \cdots \square G_n$ is the Cartesian product of connected graphs $G_1, G_2, \ldots, G_n$. Moreover, let $k \in \{1, \ldots, n\}$ and let $f = uv$ be an edge of G such that $e = u_k v_k \in E(G_k)$. Then,*

$$\begin{aligned} N_u(f|G) &= \{x \in V(G) \mid x_k \in N_{u_k}(e|G_k)\}, \\ N_v(f|G) &= \{x \in V(G) \mid x_k \in N_{v_k}(e|G_k)\}, \\ N_0(f|G) &= \{x \in V(G) \mid x_k \in N_0(e|G_k)\}. \end{aligned}$$

Proof. First, we introduce the following notation:

$$\begin{aligned} A &= \{x \in V(G) \mid x_k \in N_{u_k}(e|G_k)\}, \\ B &= \{x \in V(G) \mid x_k \in N_{v_k}(e|G_k)\}, \\ C &= \{x \in V(G) \mid x_k \in N_0(e|G_k)\}. \end{aligned}$$

We now prove that $A \subseteq N_u(f|G)$. Therefore, let $x \in A$. By (4), we know that

$$d_G(x, u) = \sum_{i=1}^{n} d_{G_i}(x_i, u_i) \text{ and } d_G(x, v) = \sum_{i=1}^{n} d_{G_i}(x_i, v_i).$$

However, $u_i = v_i$ for any $i \in \{1, \ldots, n\} \setminus \{k\}$. Hence, $d_{G_i}(x_i, u_i) = d_{G_i}(x_i, v_i)$ for all $i \in \{1, \ldots, n\} \setminus \{k\}$. On the other hand, we know that $x_k \in N_{u_k}(e|G)$, so $d_{G_k}(x_k, u_k) < d_{G_k}(x_k, v_k)$. Consequently, $d_G(x, u) < d_G(x, v)$, which also implies $x \in N_u(f|G)$. We have proved that $A \subseteq N_u(f|G)$. Analogously, one can also show that $B \subseteq N_v(f|G)$ and $C \subseteq N_0(f|G)$. Since $A \cup B \cup C = N_u(f|G) \cup N_v(f|G) \cup N_0(f|G) = V(G)$, we finally obtain

$$A = N_u(f|G), \quad B = N_v(f|G), \quad \text{and} \quad C = N_0(f|G).$$

□

We can now determine the cardinalities of the sets from Proposition 7. Note that the next corollary represents a generalization of a result from [24] to Cartesian products with more than two factors.

Corollary 1. *Suppose that $G = G_1 \square G_2 \square \cdots \square G_n$ is the Cartesian product of connected graphs $G_1, G_2, \ldots, G_n$. Moreover, let $k \in \{1, \ldots, n\}$ and let $f = uv \in E(G)$ be an edge such that $e = u_k v_k \in E(G_k)$. Then,*

$$\begin{aligned} n_u(f|G) &= |V(G/G_k)| \cdot n_{u_k}(e|G_k), \\ n_v(f|G) &= |V(G/G_k)| \cdot n_{v_k}(e|G_k), \\ n_0(f|G) &= |V(G/G_k)| \cdot n_0(e|G_k). \end{aligned}$$

Proof. By Proposition 7, we know that

$$\begin{aligned} N_u(f|G) &= \{x \in V(G) \mid x_k \in N_{u_k}(e|G_k)\} \\ &= V(G_1) \times \cdots \times V(G_{k-1}) \times N_{u_k}(e|G_k) \times V(G_{k+1}) \times \cdots \times V(G_n). \end{aligned}$$

Therefore,

$$\begin{aligned} n_u(f|G) &= |N_u(f|G)| \\ &= |V(G_1) \times \cdots \times V(G_{k-1}) \times V(G_{k+1}) \times \cdots \times V(G_n)| \cdot |N_{u_k}(e|G_k)| \\ &= |V(G_1 \square \cdots \square G_{k-1} \square G_{k+1} \square \cdots \square G_n)| \cdot |N_{u_k}(e|G_k)| \\ &= |V(G/G_k)| \cdot n_{u_k}(e|G_k), \end{aligned}$$

which completes the first part of the proof. The proofs for $n_v(f|G)$ and $n_0(f|G)$ are similar. □

In the following theorem, we show how to calculate the SMP polynomial of the Cartesian product.

Theorem 2. *Suppose that $G = G_1 \square G_2 \square \cdots \square G_n$ is the Cartesian product of connected graphs $G_1, G_2, \ldots, G_n$. Then,*

$$SMP(G;x,y) = \sum_{k=1}^{n} |V(G/G_k)| \cdot SMP\Big(G_k; x^{|V(G/G_k)|}, y^{|V(G/G_k)|}\Big).$$

Proof. In this proof, the polynomial $SMP(G;x,y)$ will be shortly denoted as SMP. Using (3) and Corollary 1, we obtain

$$\begin{aligned}
SMP &= \sum_{\substack{f=uv\in E(G),\\ n_u(f|G)\geq n_v(f|G)}} x^{n_u(f|G)} y^{n_v(f|G)} \\
&= \sum_{k=1}^{n} \sum_{\substack{f=uv\in E_k(G),\\ n_u(f|G)\geq n_v(f|G)}} x^{n_u(f|G)} y^{n_v(f|G)} \\
&= \sum_{k=1}^{n} \sum_{\substack{f=uv\in E_k(G),\\ n_{u_k}(u_kv_k|G_k)\geq n_v(u_kv_k|G_k)}} x^{|V(G/G_k)|\cdot n_{u_k}(u_kv_k|G_k)} y^{|V(G/G_k)|\cdot n_{v_k}(u_kv_k|G_k)} \\
&= \sum_{k=1}^{n} |V(G/G_k)| \cdot \sum_{\substack{e=u_kv_k\in E(G_k),\\ n_{u_k}(e|G_k)\geq n_v(e|G_k)}} x^{|V(G/G_k)|\cdot n_{u_k}(e|G_k)} y^{|V(G/G_k)|\cdot n_{v_k}(e|G_k)} \\
&= \sum_{k=1}^{n} |V(G/G_k)| \cdot \sum_{\substack{e=u_kv_k\in E(G_k),\\ n_{u_k}(e|G_k)\geq n_v(e|G_k)}} \Big(x^{|V(G/G_k)|}\Big)^{n_{u_k}(e|G_k)} \Big(y^{|V(G/G_k)|}\Big)^{n_{v_k}(e|G_k)} \\
&= \sum_{k=1}^{n} |V(G/G_k)| \cdot SMP\Big(G_k; x^{|V(G/G_k)|}, y^{|V(G/G_k)|}\Big),
\end{aligned}$$

which completes the proof. □

In the rest of the section, we investigate the edge-SMP polynomial. Here, the situation is more complicated. Firstly, we investigate some subsets of edges in Cartesian products.

Proposition 8. *Suppose that $G = G_1 \square G_2 \square \cdots \square G_n$ is the Cartesian product of connected graphs $G_1, G_2, \ldots, G_n$. Moreover, let $k \in \{1, \ldots, n\}$ and let $f = uv$ be an edge of G such that $e = u_kv_k \in E(G_k)$. Then,*

$$\begin{aligned}
M_u(f|G) &= \big\{ab \in E(G) \mid a_kb_k \in M_{u_k}(e|G_k)\big\} \cup \big\{ab \in E(G) \mid a_k = b_k \in N_{u_k}(e|G_k)\big\}, \\
M_v(f|G) &= \big\{ab \in E(G) \mid a_kb_k \in M_{v_k}(e|G_k)\big\} \cup \big\{ab \in E(G) \mid a_k = b_k \in N_{v_k}(e|G_k)\big\}, \\
M_0(f|G) &= \{ab \in E(G) \mid a_kb_k \in M_0(e|G_k)\} \cup \{ab \in E(G) \mid a_k = b_k \in N_0(e|G_k)\}.
\end{aligned}$$

Proof. We introduce the following notation:

$$\begin{aligned}
A &= \big\{ab \in E(G) \mid a_kb_k \in M_{u_k}(e|G_k)\big\} \cup \big\{ab \in E(G) \mid a_k = b_k \in N_{u_k}(e|G_k)\big\}, \\
B &= \big\{ab \in E(G) \mid a_kb_k \in M_{v_k}(e|G_k)\big\} \cup \big\{ab \in E(G) \mid a_k = b_k \in N_{v_k}(e|G_k)\big\}, \\
C &= \{ab \in E(G) \mid a_kb_k \in M_0(e|G_k)\} \cup \{ab \in E(G) \mid a_k = b_k \in N_0(e|G_k)\}.
\end{aligned}$$

Next, we prove that $A \subseteq M_u(f|G)$. First, let $ab \in E(G)$ such that $a_k b_k \in M_{u_k}(e|G_k)$, which means $d_{G_k}(a_k b_k, u_k) < d_{G_k}(a_k b_k, v_k)$. Obviously,

$$d_G(ab, u) = \min\{d_G(a, u), d_G(b, u)\} = \min\left\{\sum_{i=1}^{n} d_{G_i}(a_i, u_i), \sum_{i=1}^{n} d_{G_i}(b_i, u_i)\right\}. \tag{8}$$

Similarly,

$$d_G(ab, v) = \min\{d_G(a, v), d_G(b, v)\} = \min\left\{\sum_{i=1}^{n} d_{G_i}(a_i, v_i), \sum_{i=1}^{n} d_{G_i}(b_i, v_i)\right\}. \tag{9}$$

We know that $a_i = b_i$ and $u_i = v_i$ for every $i \in \{1, \ldots, n\} \setminus \{k\}$. Therefore, $d_{G_i}(a_i, u_i) = d_{G_i}(b_i, u_i) = d_{G_i}(a_i, v_i) = d_{G_i}(b_i, v_i)$ for any $i \in \{1, \ldots, n\} \setminus \{k\}$. As a consequence,

$$d_G(ab, u) < d_G(ab, v)$$

if and only if

$$\min\{d_{G_k}(a_k, u_k), d_{G_k}(b_k, u_k)\} < \min\{d_{G_k}(a_k, v_k), d_{G_k}(b_k, v_k)\},$$

which is equivalent to $d_{G_k}(a_k b_k, u_k) < d_{G_k}(a_k b_k, v_k)$. The last statement is true by assumption, so it follows that $d_G(ab, u) < d_G(ab, v)$ and, therefore, $ab \in M_u(f|G)$.

Next, suppose that $ab \in E(G)$ such that $a_k = b_k = N_{u_k}(e|G_k)$. Then, $d_{G_k}(a_k, u_k) < d_{G_k}(a_k, v_k)$. Moreover, there exists $j \in \{1, \ldots, n\} \setminus \{k\}$ such that $a_j b_j \in E(G_j)$, and $a_i = b_i$ for every $i \in \{1, \ldots, n\} \setminus \{j\}$. Since the distances $d_G(ab, u)$ and $d_G(ab, v)$ can be calculated as stated in (8) and (9), we observe that

$$d_G(ab, u) < d_G(ab, v)$$

if and only if

$$\begin{aligned} & \min\{d_{G_k}(a_k, u_k) + d_{G_j}(a_j, u_j), d_{G_k}(b_k, u_k) + d_{G_j}(b_j, u_j)\} \\ < \; & \min\{d_{G_k}(a_k, v_k) + d_{G_j}(a_j, v_j), d_{G_k}(b_k, v_k) + d_{G_j}(b_j, v_j)\}, \end{aligned}$$

which is equivalent to

$$\begin{aligned} & \min\{d_{G_k}(a_k, u_k) + d_{G_j}(a_j, u_j), d_{G_k}(a_k, u_k) + d_{G_j}(b_j, u_j)\} \\ < \; & \min\{d_{G_k}(a_k, v_k) + d_{G_j}(a_j, u_j), d_{G_k}(a_k, v_k) + d_{G_j}(b_j, u_j)\} \end{aligned}$$

and the last relation is further equivalent to $d_{G_k}(a_k, u_k) < d_{G_k}(a_k, v_k)$. The last statement is true by assumption, so it follows that $d_G(ab, u) < d_G(ab, v)$ and, therefore, $ab \in M_u(f|G)$. With this, we have shown that $A \subseteq M_u(f|G)$.

In a similar way, one can also show that $B \subseteq M_v(f|G)$ and $C \subseteq M_0(f|G)$. Since $A \cup B \cup C = M_u(f|G) \cup M_v(f|G) \cup M_0(f|G) = E(G)$, it follows that

$$A = M_u(f|G), \quad B = M_v(f|G), \quad \text{and} \quad C = M_0(f|G).$$

$\square$

Similarly as before, we now consider the cardinalities of the sets from Proposition 8. Again, the following corollary represents a generalization of a result from [24] to Cartesian products with more than two factors.

Corollary 2. *Suppose that $G = G_1 \square G_2 \square \cdots \square G_n$ is the Cartesian product of connected graphs $G_1, G_2, \ldots, G_n$. Moreover, let $k \in \{1, \ldots, n\}$ and let $f = uv \in E(G)$ be an edge such that $e = u_k v_k \in E(G_k)$. Then,*

$$\begin{aligned} m_u(f|G) &= |V(G/G_k)| \cdot m_{u_k}(e|G_k) + |E(G/G_k)| \cdot n_{u_k}(e|G_k), \\ m_v(f|G) &= |V(G/G_k)| \cdot m_{v_k}(e|G_k) + |E(G/G_k)| \cdot n_{v_k}(e|G_k), \\ m_0(f|G) &= |V(G/G_k)| \cdot m_0(e|G_k) + |E(G/G_k)| \cdot n_0(e|G_k). \end{aligned}$$

Proof. By Proposition 8, we know that

$$M_u(f|G) = \{ab \in E(G) \mid a_k b_k \in M_{u_k}(e|G_k)\} \cup \{ab \in E(G) \mid a_k = b_k \in N_{u_k}(e|G_k)\}.$$

Therefore, we separately consider each of the two sets on the right-hand side of the above equation. We use the following notation:

$$\begin{aligned} M_1 &= \{ab \in E(G) \mid a_k b_k \in M_{u_k}(e|G_k)\}, \\ M_2 &= \{ab \in E(G) \mid a_k = b_k \in N_{u_k}(e|G_k)\}. \end{aligned}$$

First, observe that, for an edge $ab \in M_1$, the vertex $a_i = b_i$ can be an arbitrary vertex of the graph G_i for $i \in \{1, \ldots, n\} \setminus \{k\}$. Therefore,

$$\begin{aligned} |M_1| &= |V(G_1) \times \cdots \times V(G_{k-1}) \times V(G_{k+1}) \times \cdots \times V(G_n)| \cdot |M_{u_k}(e|G_k)| \\ &= |V(G/G_k)| \cdot m_{u_k}(e|G_k). \end{aligned}$$

On the other hand, for any edge $ab \in M_2$, there exists exactly one $j \in \{1, \ldots, n\} \setminus \{k\}$ such that $a_j b_j \in E(G_j)$. Moreover, $a_k = b_k$ is a vertex from $N_{u_k}(e|G_k)$, and $a_i = b_i$ is a vertex of G_i for $i \in \{1, \ldots, n\} \setminus \{j, k\}$. Therefore, by using the second part of (7), the cardinality of the set M_2 can be computed as follows:

$$\begin{aligned} |M_2| &= |N_{u_k}(e|G_k)| \cdot \sum_{\substack{j=1 \\ j \neq k}}^{n} \left(|E(G_j)| \cdot \prod_{\substack{i=1 \\ i \neq j,k}}^{n} |V(G_i)| \right) \\ &= n_{u_k}(e|G_k) \cdot |E(G/G_k)|. \end{aligned}$$

Since the sets M_1 and M_2 are disjoint, we finally obtain

$$m_u(f|G) = |M_u(f|G)| = |M_1| + |M_2| = |V(G/G_k)| \cdot m_{u_k}(e|G_k) + |E(G/G_k)| \cdot n_{u_k}(e|G_k),$$

which completes the first part of the proof. The proofs for $m_v(f|G)$ and $m_0(f|G)$ are analogous. □

Let $G = G_1 \square G_2 \square \cdots \square G_n$ be the Cartesian product of connected graphs $G_1, G_2, \ldots, G_n$ and let $k \in \{1, \ldots, n\}$. For any edge $e = u_k v_k \in E(G_k)$, we introduce the following notation:

$$\begin{aligned} \alpha_{u_k}(e|G_k) &= |V(G/G_k)| \cdot m_{u_k}(e|G_k) + |E(G/G_k)| \cdot n_{u_k}(e|G_k), \\ \alpha_{v_k}(e|G_k) &= |V(G/G_k)| \cdot m_{v_k}(e|G_k) + |E(G/G_k)| \cdot n_{v_k}(e|G_k). \end{aligned}$$

Moreover, we define the edge-weights $w_1^k(e)$ and $w_2^k(e)$ for an edge $e = u_k v_k$ of the graph G_k as

$$w_1^k(e) = \max\{\alpha_{u_k}(e|G_k), \alpha_{v_k}(e|G_k)\} \text{ and } w_2^k(e) = \min\{\alpha_{u_k}(e|G_k), \alpha_{v_k}(e|G_k)\}. \tag{10}$$

Using the above notation, we can now express the edge-SMP polynomial of the Cartesian product G by the weighted SMP polynomials of factors $G_1, G_2, \ldots, G_n$.

Theorem 3. *Suppose that $G = G_1 \square G_2 \square \cdots \square G_n$ is the Cartesian product of connected graphs $G_1, G_2, \ldots, G_n$. Then,*

$$SMP_e(G; x, y) = \sum_{k=1}^{n} |V(G/G_k)| \cdot SMP_{(w_1^k, w_2^k)}(G_k; x, y),$$

where the weights w_1^k, w_2^k are defined in (10).

Proof. Using (3), we obtain

$$\begin{aligned} SMP_e(G; x, y) &= \sum_{\substack{f = uv \in E(G), \\ m_u(f|G) \geq m_v(f|G)}} x^{m_u(f|G)} y^{m_v(f|G)} \\ &= \sum_{k=1}^{n} \sum_{\substack{f = uv \in E_k(G), \\ m_u(f|G) \geq m_v(f|G)}} x^{m_u(f|G)} y^{m_v(f|G)}. \end{aligned}$$

If $k \in \{1, \ldots, n\}$ and $f = uv \in E_k(G)$, then, by Corollary 2, we know that $m_u(f|G) = \alpha_{u_k}(e|G_k)$ and $m_v(f|G) = \alpha_{v_k}(e|G_k)$, where $e = u_k v_k \in E(G_k)$. Therefore, by (10) and (2), we obtain

$$\begin{aligned} SMP_e(G; x, y) &= \sum_{k=1}^{n} \sum_{f = uv \in E_k(G)} x^{w_1^k(u_k v_k)} y^{w_2^k(u_k v_k)} \\ &= \sum_{k=1}^{n} |V(G/G_k)| \cdot \sum_{e = u_k v_k \in E(G_k)} x^{w_1^k(e)} y^{w_2^k(e)} \\ &= \sum_{k=1}^{n} |V(G/G_k)| \cdot SMP_{(w_1^k, w_2^k)}(G_k; x, y). \end{aligned}$$

□

Note that, by Theorems 2 and 3, one can compute the (edge-)SMP polynomial of the Cartesian product $G = G_1 \square G_2 \square \cdots \square G_n$ by using its factors. The numbers $|V(G/G_k)|$ and $|E(G/G_k)|$, $k \in \{1, \ldots, n\}$ that appear in these statements can be instantly calculated using (7).

5. Conclusions

In the present paper, we defined the SMP polynomial of a graph. This polynomial has two variables and can be used to calculate three important topological indices: the Szeged index, the Mostar index, and the vertex-PI index. Similarly, the edge-SMP polynomial was introduced. Then, some properties of these polynomials were stated for bipartite graphs, trees, cycles, complete graphs, and edge-transitive graphs. Moreover, bounds on the degrees of these two polynomials were investigated and several open problems were proposed. Furthermore, we focused on the SMP polynomials of Cartesian products. Several auxiliary statements related to some subsets of vertices and edges in Cartesian products of graphs were firstly deduced. Based on these results, formulas for calculating SMP polynomials of a Cartesian product of graphs from its factors were finally provided.

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