

Scientific paper

Omega Polynomial Revisited

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This paper is dedicated to Professor Milan Randić on the occasion of his 80th birthday

Abstract

Omega polynomial was proposed by Diudea (Omega Polynomial, *Carpath. J. Math.*, **2006**, 22, 43–47) to count the opposite topologically parallel edges in graphs, particularly to describe the polyhedral nanostructures. In this paper, the main definitions are re-analyzed and clear relations with other three related polynomials are established. These relations are supported by close formulas and appropriate examples.

Keywords: Counting polynomials: Omega, Theta, Pi, Sadhana; Cluj-Ilmenau CI index

1. Introduction

Recently several graph polynomials were introduced in mathematical chemistry to give further insights into the structure and properties of chemical graphs. In particular, the first derivative of such polynomials computed at a given value returns a corresponding topological index of interest.

A graph polynomial, also called a counting polynomial, can be written as

$P(G,x) = \sum_k m(G,k) \cdot x^k$, with the exponents showing the extent of partitions $p(G)$, $\cup p(G) = P(G)$ of a graph property $P(G)$ while the coefficients $m(G,k)$ are related to the number of partitions of extent k .

Counting polynomials have been introduced, in the Mathematical Chemistry literature, by Hosoya,^{1,2} to count independent edge sets (the Z-polynomial) and the distances in the graph (the Wiener polynomial, latter called the Hosoya polynomial and denoted $H(G,x)$).^{3,4} The same author also proposed the sextet polynomial^{5,6} to count the resonant rings in a benzenoid molecule. Other counting polynomials are the *independence* polynomial,^{7–9} *domino*,¹⁰ *star*,¹¹ and *clique*¹² polynomials. More about polynomials the reader can find in ref.¹³

Some distance-related properties can be expressed

in polynomial form, with coefficients calculable from the layer and shell matrices.^{14–17} These matrices are built up according to the vertex distance partitions of a graph, as provided by the TOPOCLUJ software package.¹⁸ The most important, in this respect, is the evaluation of the coefficients of Hosoya $H(G,x)$ polynomial from the layer of counting (LC) matrix. The aim of this paper is to give a unified approach to these polynomials and invariants and to give links to the existing concepts in pure mathematics.

2. Relation *co* and Its Relatives

Let $G=(V(G),E(G))$ be a connected graph, with the vertex set $V(G)$ and edge set $E(G)$. Two edges $e = uv$ and $f = xy$ of G are called *codistant* (briefly: *e cof*) if the notation can be selected such that¹⁹

$$d(v,x) = d(v,y) + 1 = d(u,x) + 1 = d(u,y), \quad (1)$$

where d is the usual shortest-path distance function. Clearly, relation *co* is reflexive, that is, $e co e$ holds for any edge e of G . Relation *co* is also symmetric: if $e cof$ then also $f co e$. On the other hand, *co* is in general non-transitive, a small example demonstrating this fact is the complete bipartite graph $K_{2,3}$ (Figure 3, with only three points

of degree 2 or with a single bent line inside the square). A graph is called a *co-graph* if the relation *co* is transitive and thus an equivalence relation. The cubic net in Figure 1, b is a *co-graph*.

For an edge $e \in E(G)$, let $C(e) = \{f \in E(G); f \text{ co } e\}$ be the set of edges in G that are codistant to e . For instance, if e is an arbitrary edge of the complete bipartite graph $K_{2,n}$, then $C(e)$ consists of all the edges that are not adjacent to e . The set $C(e)$ is called an *orthogonal cut* (*oc* for short) of G (with respect to e). If G is a *co-graph* then its orthogonal cuts C_1, C_2, \dots, C_k form a partition of $E(G)$: $E(G) = C_1 \cup C_2 \cup \dots \cup C_k$, $C_i \cap C_j = \emptyset$, $i \neq j$.

Let us first turn the attention to bipartite graphs. To state several characterizations of bipartite *co-graphs*, further definitions are needed.

A subgraph $H \subseteq G$ is called *isometric*, if $d_H(u,v) = d_G(u,v)$, for any $(u,v) \in H$; it is *convex* if any shortest path in G between vertices of H belongs to H . The n -cube Q_n is the graph whose vertices are all binary strings of length n , two strings being adjacent if they differ in exactly one position.²⁰ (Note that the distance function in the n -cube is just the Hamming distance: the distance between two vertices of Q_n is equal to the number of positions in which they differ.) A graph G is called a *partial cube* if there exists an integer n such that G is an isometric subgraph of Q_n .

For any edge ab of a connected graph G let W_{ab} denote the set of vertices lying closer to a than to b : $W_{ab} = \{w \in V(G) | d(w,a) < d(w,b)\}$. It follows from the definition that $W_{ab} = \{w \in V(G) | d(w,b) = d(w,a) + 1\}$. We will use W_{ab} also to denote a subgraph induced by these vertices. Then the sets (and subgraphs) W_{ab} are called *semicubes* of G . The *semicubes* W_{ab} and W_{ba} are *opposite semicubes*. Clearly, two opposite *semicubes* are disjoint. Moreover, a graph G is bipartite if and only if, for any edge of G , the opposite *semicubes* form a partition of $V(G)$.

Finally, let G be a connected graph and $e = uv$ and $f = xy$ edges of G . Then $e \Theta f$ if $d(u,x) + d(v,y) \neq d(u,y) + d(v,x)$. Now everything is defined for the following result.

THEOREM 1. The following statements are equivalent for a bipartite graph G :

- (i) G is a *co graph*;
- (ii) G is a *partial cube*;
- (iii) All *semicubes* of G are *convex*;
- (iv) Relation Θ is *transitive*.

Equivalence between (i) and (ii) was observed by Klavžar,²¹ equivalence between (ii) and (iii) is due to Djoković,²² while the equivalence between (ii) and (iv) was proved by Winkler.²³

Let us return to arbitrary (that is, not necessary bipartite) connected graphs. Let $e = uv$ and $f = xy$ be two edges of a connected graph G . Then Djoković²² defined relation \sim on $E(G)$ by setting $e \sim f$ if f joins a vertex in W_{xy} with a vertex in W_{yx} . For more information on the relation \sim see refs.^{24,25}

LEMMA 1. In any connected graph, $co = \sim$.

Proof. Let $e = uv$ and $f = xy$ be edges of a connected graph G . Suppose first $e \text{ co } f$, that is, $d(x,u) = d(v,y) + 1 = d(u,x) + 1 = d(u,y)$. Since $d(x,u) < d(x,v)$, $x \in W_{vu}$ and since $d(y,v) < d(y,u)$, $y \in W_{vu}$. Thus, $e \sim f$. Suppose $e \sim f$, with $x \in W_{vu}$ and $y \in W_{vu}$. Then $d(v,x) = d(v,y) + d(u,x) = d(u,x) + 1$ and $d(u,y) = d(u,v) + d(v,y) = 1 + d(v,y)$. Since $d(u,x) = d(v,y)$ we conclude that $e \text{ co } f$. Q.E.D.

In general $\sim \subseteq \Theta$ and in bipartite graphs $\sim = \Theta$. Hence the above discussion can be briefly summarized as follows:

PROPOSITION 1. Let G be a connected graph; then $co = \sim$. If G is also bipartite, then $co = \sim = \Theta$.

3. Four Counting Polynomials

Relation *co* is a particular case of the edge *equidistance* (*eqd*) relation. The equidistance of two edges $e = uv$ and $f = xy$ in a connected graph G is described in part by relation (1), (accounting for topologically parallel edges), to which the condition for topologically perpendicular edges (in tetrahedron and its extensions) must be added:

$$d(u,x) = d(u,y) = d(v,x) = d(v,y), \text{ for } \perp \text{ edges} \quad (2)$$

Notice that Ashrafi defined the equidistance of edges by considering the distance from a vertex z to an edge $e = uv$ as the minimum distance between the given point and the two endpoints of that edge:^{26,27} $d(z,e) = \min\{d(z,u), d(z,v)\}$. Then, the edges $e = uv$ and $f = xy$ are equidistant if

$$d(x,e) = d(y,e) \text{ and } d(u,f) = d(v,f) \quad (3)$$

In tetrahedron and its extensions, relation (3) is still true but in general it is not.

Recall that a graph is *planar* if it allows an embedding into the plane such that no two edges cross. A planar graph together with its fixed embedding into the plane is called a *plane graph*. In chemistry, not only the structure of a chemical graph but also its geometry is important. Most of the chemical graphs are by their nature planar (and most often also equipped with an embedding into the plane). Moreover, the natural embeddings of these graphs are such that all the inner faces are isometric cycles which we will assume in the following. Hence the following definitions are relevant in this context.

We say that edges e and f of a plane graph G are in relation *opposite*, $e \text{ op } f$, if they are opposite edges of an inner face of G . Then $e \text{ co } f$ holds by the assumption that faces are isometric. Notice that the relation *co* is defined in the whole graph while *op* is defined only in faces. We mention that John *et al.*^{19,28} implicitly used the “*op*” relation in defining the Cluj-Ilmenau index *CI* (see below).

Using the relation *op* we can partition the edge set of G into *opposite edge strips (ops)* for short, as follows.

1. Any two subsequent edges of an *ops* are in *op* relation.
2. Any three subsequent edges of such a strip belong to adjacent faces.
3. An *ops* starts/ends in either (i) one even face/ring or (ii) two odd faces/rings; in case (i), the *ops* is a cycle while in case (ii) it is a path. In case of open structures, the open (or infinite) faces are equivalent to the odd faces. There are cases in which the two odd faces/rings superimpose and *ops* is a *pseudo cycle*, because the *op* relation is lastly violated.^{29,30}

The *ops* is taken as maximum possible, irrespective of the starting edge. The choice is about the maximum size of face/ring, and mode of face/ring counting, which will decide the length of the strip.

Let G be an arbitrary connected graph and s_1, s_2, \dots, s_k be the *op*-strips of G . Then *ops* form a partition of $E(G)$ and the Ω -polynomial³¹ of G is defined as

$$\Omega(G, x) = \sum_{i=1}^k x^{|S_i|} \quad (4)$$

Let now the set of edges codistant to edge e of G be $C(e)$. A Θ -polynomial³² of G , counting the edges equidistant to the all reference edges e , is written as

$$\Theta(G, x) = \sum_{e \in E(G)} x^{|C(e)|} \quad (5)$$

Suppose now G is a *co*-graph; then

$$\begin{aligned} \Theta(G, x) &= \sum_{e \in E(G)} x^{|C(e)|} = \sum_{i=1}^k \sum_{e \in S_i} x^{|C(e)|} \\ &= \sum_e |C(e)| x^{|C(e)|} = \sum_{i=1}^k |S_i| x^{|S_i|} \end{aligned} \quad (6)$$

If the polynomial counts the edges non-equidistant to the all reference edges e , it is called the Π -polynomial³² and is defined as

$$\Pi(G, x) = \sum_{e \in E(G)} x^{|E(G)| - |C(e)|} = \sum_{i=1}^k |S_i| x^{|E(G)| - |S_i|} \quad (7)$$

A fourth polynomial also related to the *ops* in G , but counting the non-opposite edges is the *Sadhana Sd* polynomial³³ defined as

$$Sd(G, x) = \sum_{i=1}^k x^{|E(G)| - |S_i|} \quad (8)$$

The first derivative (computed at $x = 1$) of these counting polynomials give interesting inter-relations and valuable information on the graph

$$\Omega'(G, 1) = \sum_{i=1}^k |S_i| = |E(G)| \quad (9)$$

$$\Theta'(G, 1) = \sum_{i=1}^k (|S_i|)^2 = \theta(G) \quad (10)$$

$$\Pi'(G, 1) = \sum_{i=1}^k |S_i| (|E(G)| - |S_i|) = \Pi(G) \quad (11)$$

$$Sd'(G, 1) = \sum_{i=1}^k (|E(G)| - |S_i|) = Sd(G) \quad (12)$$

On $\Omega(G, x)$ an index, called Cluj-Ilmenau¹⁹ $CI(G)$, is defined

$$CI(G) = \{[\Omega'(G, 1)]^2 - [\Omega'(G, 1) + \Omega''(G, 1)]\} \quad (13)$$

The sum of the first derivative (in $x = 1$) of the polynomials counting equidistant *eqd* and non-equidistant *neqd* edges in G is square of the number of edges in G or

$$\Theta'(G, 1) + \Pi'(G, 1) = (\Omega'(G, 1))^2 = (|E(G)|)^2 \quad (14)$$

while the value of these polynomials in $x = 1$ is

$$\Theta(G, 1) = \Pi(G, 1) = \Omega'(G, 1) = |E(G)| \quad (15)$$

The first derivative (in $x = 1$) of *Sadhana* polynomial equals the *Sadhana index*³⁴ and is a multiple of $|E(G)|$:

$$\begin{aligned} Sd'(G, 1) &= \sum_{i=1}^k (|E(G)| - |s_i|) = \\ &= |E(G)| (|ops(G)| - 1) \end{aligned} \quad (16)$$

Since $|ops(G)| = \Omega(G, 1) = Sd(G, 1)$, and considering (9), the relation³⁵ of *Sadhana index* with *Omega* polynomial, out of the basic definition, is

$$Sd'(G, 1) = \Omega'(G, 1)(\Omega(G, 1) - 1) \quad (17)$$

PROPOSITION 2. In bipartite *co*-graphs, $CI(G) = \Pi(G)$.

Proof. By the definition of CI ,

$$\begin{aligned} CI(G) &= \left(\sum_{i=1}^k |S_i| \right)^2 - \left(\sum_{i=1}^k |S_i| + \sum_{i=1}^k |S_i| (|S_i| - 1) \right) \\ &= |E(G)|^2 - \sum_{i=1}^k (|S_i|)^2 = \Pi'(G, 1) = \Pi(G) \end{aligned} \quad (18)$$

Only in bipartite *co*-graphs, $\Pi(G)$ equals the value of Π (Padmakar-Ivan) index,³⁶ proposed by Khadikar to account for the sum of non-equidistant edges in G . In ge-

neral, $CI(G) \neq \Pi(G) \neq PI(G)$, because the edge equidistance *eqd* relation includes, besides the parallel edges condition (*co* and *op* relations), also the condition for perpendicular edges (tetrahedron condition).

From the above relations (9), (10) and (18), one can reformulate (11) as

$$\begin{aligned} \Pi(G) &= |E(G)|^2 - \sum_{i=1}^k (|S_i|)^2 = \\ &= \{[\Omega'(G, 1)]^2 - \Theta'(G, 1)\} \end{aligned} \quad (19)$$

Relation (19) is just the formula proposed by John *et al.*²⁸ to calculate the Khadikar's *PI* index.

4. Examples

(a) There exist plane bipartite graphs, which are *co*-graphs and for which $CI(G) = \Pi(G)$. It is the case of acenes and phenacenes, which are polyhex molecular structures. For these classes of structures, analytical formulas were presented in ref.³² Formulas for other classes of polyhex plane graphs, such as phenylenes, spiranes, pyrenes and coronenes were given in ref.³⁷

(b) There exist planar 3D bipartite graphs, which are non *co*-graphs and for which $CI(G) \neq \Pi(G)$. An example is the cage in Figure 1a: the red edges are non-equidistant

to each other although they both belong to the same *ops*. Conversely, the *pcu* cubic lattice in Figure 1b is precisely a partial cube (also a *co*-graph) and their *ops* represent orthogonal cuts *oc*; thus $CI(G) = \Pi(G)$ (shaded values).

To the list of non *co*-graphs which are 3D bipartite graphs, we add the toroidal lattices of even faces. Only exceptional tori show $CI(G) = \Pi(G)$ values (Table 1).

The tori of entries 1 and 2 of Table 1 are 3D bipartite graphs and show $CI(G) = \Pi(G)$ values, although they do not follow the relations (6) and (7) for $\Pi(G, x)$ and $\Theta(G, x)$.³⁸ The structure in entry 3 is a non-bipartite graph³² as the whole; however, it represents a union of three strips, each of them being a bipartite, *co*-graph (Figure 2). As a consequence, the relations (6) and (7) are obeyed. Note that, in Ref.³⁷ $\Pi(G, x)$ was denoted by $N\Omega(G, x)$. The polynomial calculations were done by the software programs developed at TOPO Group Cluj: Omega Counter³⁹ and Nano Studio.⁴⁰

(c) In tree graphs, Omega polynomial simply counts the non-equidistant edges as self-equidistant ones, being included in the term of exponent $s = 1$. In such graphs, $CI(G) = \Pi(G) = (v - 1)(v - 2)$ (a result known from Khadikar⁴¹) and the Omega and Theta polynomials show the same expression.

(d) Finally, there are graphs with a single *ops*, which is precisely a *cycle* (called a Hamiltonian *ops* in ref.²⁹).

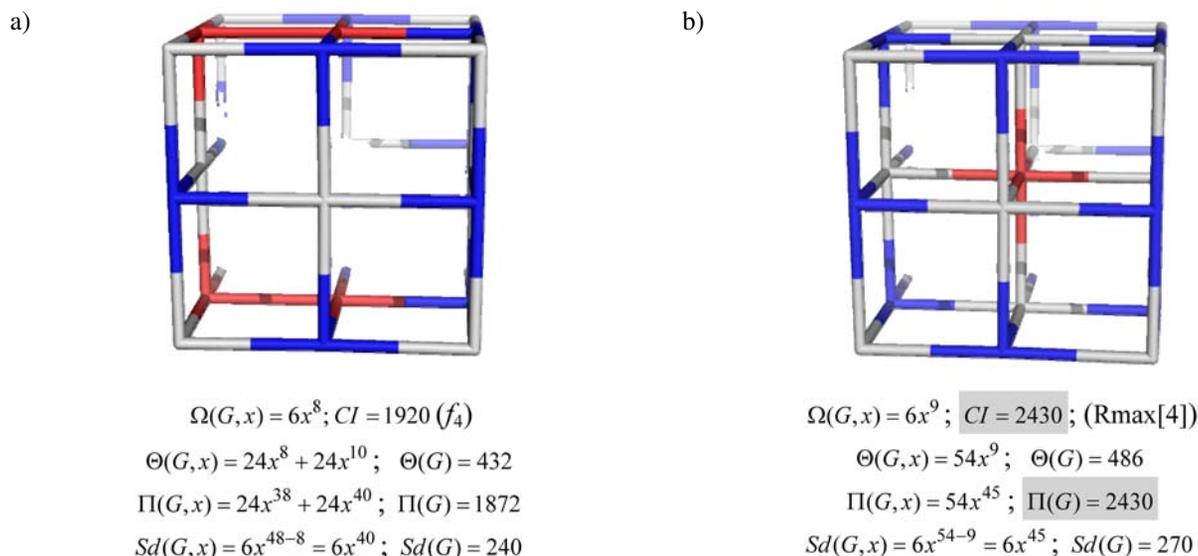


Figure 1. 3D bipartite graphs; (a) non-*co*-graph and (b) *co*-graph (gray marked $CI(G) = \Pi(G)$ values)

Table 1. Polynomials in toroidal structures, for which $CI(G) = \Pi(G)$.

	Torus	$\Omega(G, x)$	CI	$\Pi(G, x)$	$\Pi(G)$	$\Theta(G, x)$
1	TH(6,3)[8,12]	$12x^4 + 4x^{24}$	18240	$96x^{122} + 48x^{136}$	18240	$48x^8 + 96x^{22}$
2	TH((4,8)3)[20,8]	$10x^8 + 8x^{10} + 2x^{40}$	52960	$80x^{218} + 80x^{220} + 80x^{224}$	52960	$80x^{16} + 80x^{20} + 80x^{22}$
3	TWV3(4,4)[6,10]	$10x^6 + 3x^{20}$	12840	$60x^{100} + 60x^{114}$	12840	$60x^6 + 60x^{20}$

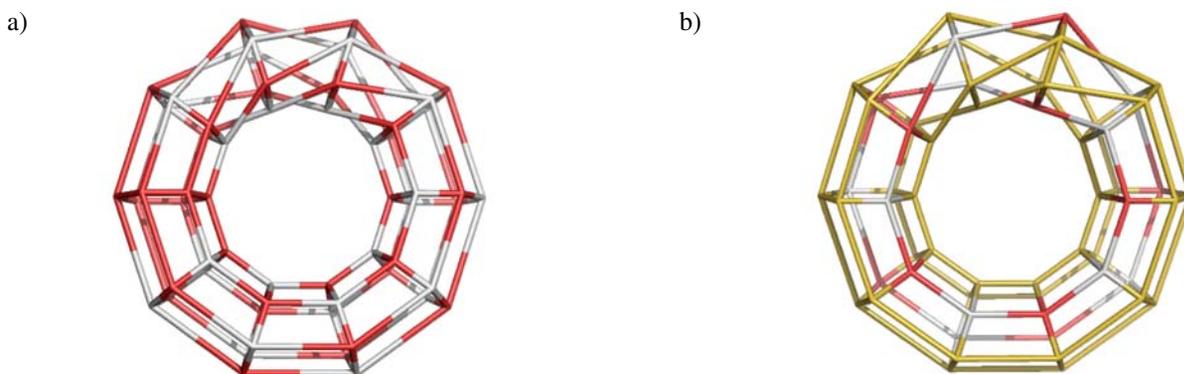
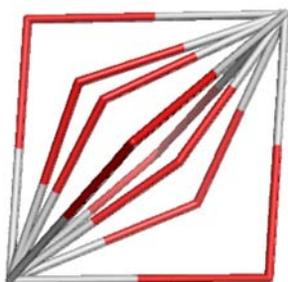


Figure 2. Twisted torus TWV3[6,10](4,4); non-bipartite (a); union of 3 *co*-graphs, one of them is shown, alternating white-red colors (b).

For such graphs, one calculates: $\Omega(G, x) = 1x$; $CI(G) = s^2 - (s + s(s - 1)) = 0$. An example is given in Figure 3.



$$\begin{aligned}\Omega(G, x) &= x^{2n} \text{ (all rings)} \\ \Omega'(G, 1) &= e = 2n \\ \Omega''(G, 1) &= 2n(2n - 1) \\ CI(G) &= 0 \\ \Theta(G, x) &= 2nx^n \\ \Theta'(G, 1) &= \Theta(G) = 2n^2 \\ \Pi(G, x) &= 2nx^{e-n} = 2nx^{2n-n} = 2nx^n \\ \Pi'(G, 1) &= \Pi(G) = 2n^2 \\ Sd(G, x) &= x^{e-2n} = x^{2n-2n} = 1 \\ Sd(G) &= 0\end{aligned}$$

Ex. For $n=5$, CI , Θ , Π , Sd : 0; 50; 50; 0.

Figure 3. A complete bipartite graph $K_{2,n}$; $n = 8$; non-*co*-graph; Hamiltonian *ops*

5. One More Question

It is natural to ask whether there is a simple criterion/condition to be used in order to decide if a given bipartite graph is a *co*-graph (or a partial cube). More precisely, one would like to have a criterion that can be applied fast either by hand or by computer. Unfortunately, no such condition is known and, in fact, such a condition would be a big breakthrough in the area of metric graph theory. In the papers,^{42,43} two algorithms of the complexity $O(mn)$

for recognizing *co*-graphs have been developed, where n is the order and m the size of a given graph. (Note that in a *co* graph, $m = O(n \log n)$.) Recently Eppstein,⁴⁴ using some sophisticated computational tricks, reduced the complexity to $O(n^2)$ thus removing the factor $\log n$. In some special cases the complexity can be further reduced, see ref.⁴⁵ but in general a (close to) linear criterion does not seem realistic.

Omega polynomial found application in the topological description of complex nanostructures showing polyhedral covering.^{46–48} In tubular/toroidal structures this polynomial accounts for the spirality and ring distribution.^{49–51} The coefficient of the first power term, called n_p , has found to have good ability in predicting the heat of formation and strain energy in small fullerenes or the resonance energy in planar benzenoids.^{37,38}

6. Conclusions.

Omega polynomial was designed to count the opposite topologically parallel edges in graphs, particularly to describe the polyhedral nanostructures. In four years, 43 papers have been published or sent for publication by TOPO Group Cluj and further papers by other scientists, Omega polynomial already getting a scientific success.

In this paper, the main definitions were re-analyzed and clear relations with other three related polynomials were established. These relations were supported by close formulas and appropriate examples.

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Povzetek

Omega polinom je predlagal Diudea (ref.: Omega Polynomial, *Carpath. J. Math.*, 22 43–47) za štetje nasprotnih topološko vzporednih povezav v grafih, še posebej za opis poliedričnih nanostruktur. V tem članku so ponovno analizirane glavne definicije in vzpostavljene jasne povezave z ostalimi tremi sorodnimi polinomi. Te povezave so podprte z izpeljanimi formulami in ustreznimi primeri.