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Original Scientific Article

Cluj CJ and PIv Polynomials

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Abstract. A parallel between the counting polynomials CJ(x) and PIv(x), proposed by the groups of Diudea (Romania) and Ashrafi (Iran), respectively, is presented. The both polynomials count the non-equidistant vertices, with respect to any edge in a graph; the difference appeared at the operational stage, as will be demonstrated in this paper. Their first derivatives, in $x = 1$, provide one and the same value; however, the second derivatives are different. Analytical relations for calculating these polynomials and their single number descriptors, in some classes of graphs are derived.

Keywords: counting polynomial, Cluj index, PI vertex index, Cluj matrix

INTRODUCTION

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.

These polynomials are useful as elegant descriptions of molecular topology, being sources of more than one index, *i.e.*, single numbers descriptors, but also providing deep inside of the molecular structure.

Counting polynomials were introduced in the Mathematical Chemistry literature by Hosoya[1,2] with his Z-counting (independent edge sets) and the distance degree (initially called Wiener and later Hosoya)[3,4] polynomials. A variety of such polynomials were further proposed: the sextet polynomial,[5,6] to count the resonant rings in a benzenoid molecule, the independence polynomial,[7–9] which counts selections of k-independent vertices in the graph, the *king*, *color*, *star* and *clique* polynomials being also included in the list.[10–13]

For some distance-related properties, the polynomial coefficients are calculable from the layer and shell matrices,[14,15] which can be built according to the vertex distance partitions of a graph, as provided by the TOPOCLUJ software package.[16]

This paper is devoted to the mathematical aspects of the Cluj polynomials in relation to the newer $\mathrm{PI_v}$ polynomial. Definitions of Cluj matrices and polynomials are provided in the next section while the $\mathrm{PI_v}$ polynomial is defined in the third section. Some more remarks on the properties of these polynomials and formulas for counting them in several classes of graphs are presented in the fourth section.

2. CLUJ MATRICES AND POLYNOMIALS

A Cluj fragment[17–20] $\mathrm{CJ}_{i,j,p}$ collects vertices v lying closer to i than to j, the endpoints of a path $p(i,j)$. Such a fragment collects the vertex proximities of i against any vertex j, joined by the path p, with the distances measured in the subgraph $D_{(G-p)}$, as shown in the following equation:

$$\mathrm{CJ}_{i,j,p} = \left\{ v \middle| v \in V(G); D_{(G-p)}(i,v) < D_{(G-p)}(j,v) \right\} \quad (1)$$

In graphs containing rings, more than one path could join the pair (i, j), thus resulting more than one fragment related to i (with respect to j and a given path p). The entries in the Cluj matrix are taken, by definition, as the maximum cardinality among all such fragments:

$$[\mathbf{UCJ}]_{i,j} = \max_p \left|\mathrm{CJ}_{i,j,p}\right| \quad (2)$$

In trees, due to the unique nature of paths joining any two vertices, $\mathrm{CJ}_{i,j,p}$ represents the set of paths going to

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j through i. In this way, the path $p(i,j)$ is characterized by a single endpoint, which is sufficient to calculate the unsymmetric matrix **UCJ**. When the path p belongs to the set of distances DI(G), the suffix DI is added to the name of matrix, as in **UCJDI**. When path p belongs to the set of detours DE(G), the suffix is DE. When the matrix symbol is not followed by a suffix, it is implicitly DI. The Cluj matrices are defined in any graph and, except for some symmetric graphs, are unsymmetric and can be symmetrized by the Hadamard multiplication with their transposes

$$\mathbf{SM}_{\mathrm{p}} = \mathbf{UM}\bullet(\mathbf{UM})^{\mathrm{T}} \tag{3}$$

If the matrices calculated from edges (*i.e.*, on adjacent vertex pairs) are required, the matrices calculated from paths must be multiplied by the adjacency matrix $\boldsymbol{A}$ (which has the non-diagonal entries of 1 if the vertices are joined by an edge and, otherwise, zero)

$$\mathbf{SM}_{\mathrm{e}} = \mathbf{SM}_{\mathrm{p}}\bullet\boldsymbol{A} \tag{4}$$

The basic properties and applications of the above matrices and derived descriptors have been presented elsewhere.[21–26] Notice that the Cluj indices, previously used in correlating studies, were calculated on the symmetric matrices, thus involving a multiplicative operation. Also, the symbol CJ (Cluj) is used for the previously denoted CF (Cluj fragmental) matrices and indices.

Our attention is here focused on the unsymmetric matrices **UCJ**, defined on distances and calculated on path $\mathbf{UCJ_p}$ and on edges $\mathbf{UCJ_e}$. Figure 1 illustrates the two matrices in the case of the graph called Ph15. The relation between the two matrices in given below

$$\mathbf{UCJ}_{\mathrm{e}} = \mathbf{UCJ}_{\mathrm{p}}\bullet\boldsymbol{A} \tag{5}$$

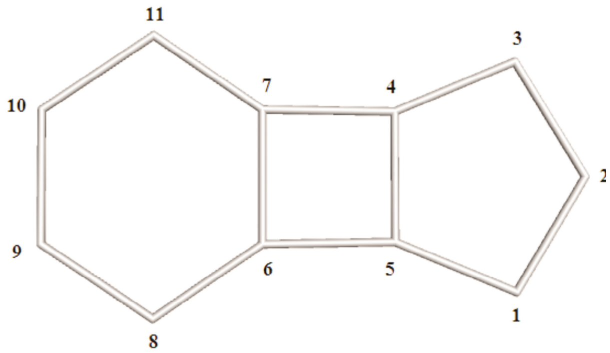
The Cluj polynomials are defined[27,28] on the basis of Cluj matrices as

$$\mathrm{CJ}(G,x) = \sum\nolimits_k m(G,k)\cdot x^k \tag{6}$$

They count the vertex proximity of the vertex i with respect to any vertex j in G, joined to i by an edge $\{p_{e,i}\}$ (the Cluj-edge polynomials) or by a path $\{p_{p,i}\}$ (the Cluj-path polynomials), taken as the shortest (*i.e.*, distance DI) or the longest (*i.e.*, detour DE) paths. In Eq. (6), the coefficients $m(G,k)$ are calculated from the entries of unsymmetric Cluj matrices. The summation runs over all $k = |\{p\}|$ in G.

The polynomial coefficients are counted from the Cluj matrices by the TOPOCLUJ software program[16] and also by a simple routine for collecting the entries in the unsymmetric matrices **UCJ**. In the case of the $\mathrm{CJ_e}$ polynomial, an orthogonal edge-cutting procedure can be used, as shown in Table 1. The same procedure has been used by Gutman and Klavžar to calculate the Szeged index of polyhex graphs.[29]

As can be seen from Table 1, the proximities of the two ends of any edge in the graph, collected from the upper/lower triangle of $\mathbf{UCJ_e}$ matrix, depend on the graph numbering, thus being variant. To make the polynomial invariant, we simply summed the two partial polynomials (Table 1, entries 1 and 2) to obtain the



Ph15

$\mathbf{UCJ_p}$(Ph15)

	1	2	3	4	5	6	7	8	9	10	11	RS
1	0	5	5	2	2	3	3	4	4	4	4	36
2	2	0	2	2	2	2	2	4	3	3	4	26
3	5	5	0	2	2	3	3	4	4	4	4	36
4	8	8	8	0	5	4	5	6	5	6	6	61
5	8	8	8	5	0	5	4	6	6	5	6	61
6	7	6	6	5	6	0	5	8	7	7	7	64
7	6	6	7	6	5	5	0	7	7	7	8	64
8	4	4	5	4	3	3	2	0	8	5	4	42
9	4	3	4	3	3	2	2	3	0	5	2	31
10	4	3	4	3	3	2	2	2	5	0	3	31
11	5	4	4	3	4	2	3	4	5	8	0	42
CS	53	52	53	35	35	31	31	48	54	54	48	494

$\mathbf{UCJ_e}$(Ph15)

	1	2	3	4	5	6	7	8	9	10	11	RS
1	0	5	0	0	2	0	0	0	0	0	0	7
2	2	0	2	0	0	0	0	0	0	0	0	4
3	0	5	0	2	0	0	0	0	0	0	0	7
4	0	0	8	0	5	0	5	0	0	0	0	18
5	8	0	0	5	0	5	0	0	0	0	0	18
6	0	0	0	0	6	0	5	8	0	0	0	19
7	0	0	0	6	0	5	0	0	0	0	8	19
8	0	0	0	0	0	3	0	0	8	0	0	11
9	0	0	0	0	0	0	0	3	0	5	0	8
10	0	0	0	0	0	0	0	0	5	0	3	8
11	0	0	0	0	0	0	3	0	0	8	0	11
CS	10	10	10	13	13	13	13	11	13	13	11	130

Figure 1. The Cluj matrix $\mathbf{UCJ_e}$ of the graph Ph15.

Table 1. Edge cut procedure in defining the CJ and PI_v polynomials

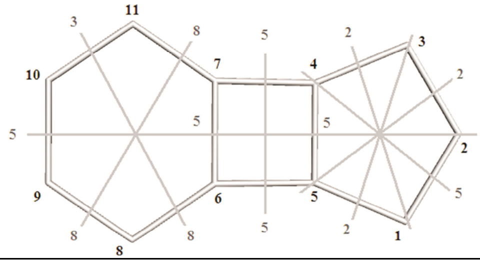
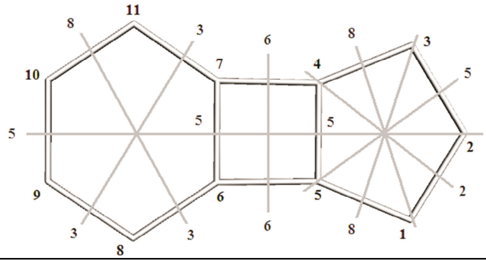
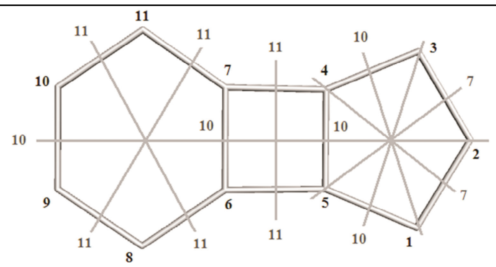
	Graph	Polynomials
1		upper triangle: *i<j* $CJ_e(x; i<j) = 3x^8 + 0x^6 + 6x^5 + 1x^3 + 3x^2$ $CJ_e(1; i<j) = \mathrm{e} = \lvert E(G) \rvert = 13$
2		lower triangle: *i>j* $CJ_e(x; i>j) = 3x^8 + 2x^6 + 4x^5 + 3x^3 + 1x^2$ $CJ_e(1; i>j) = \mathrm{e} = 13$
3	Global polynomial $CJ_e(x) = 6x^8 + 2x^6 + 10x^5 + 4x^3 + 4x^2$ $CJ_e(1) = 2e = 26$ $CJ_e'(1) = 130$ $CJ_e''(1) = 628$	$J_p(x) = 10x^8 + 8x^7 + 12x^6 + 20x^5 + 24x^4 + 18x^3 + 18x^2$ $J_p(1) = 2p = 110$ $J_p'(1) = 494$
4		$PI_v(x) = 6x^{11} + 5x^{10} + 2x^7$ $\mathrm{v} = \lvert V(G) \rvert = 11$ $PI_v(1) = \mathrm{e} = 13$ $PI_v'(1) = PI_v = 130$ $PI_v''(1) = 1194$

Table 2. Edge cut procedure for calculating CJ and PI_v polynomials in a bipartite graph

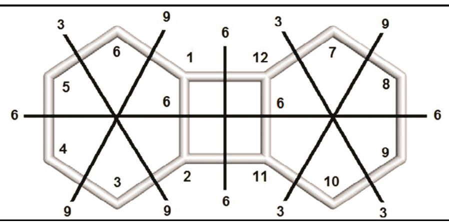
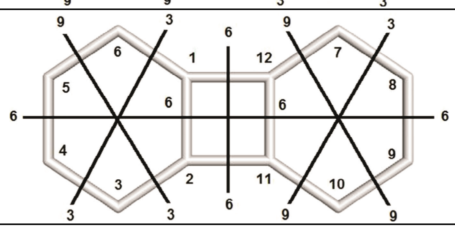
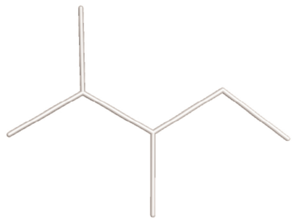
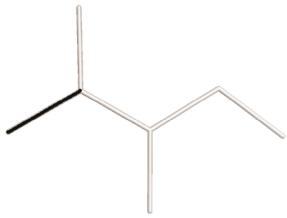
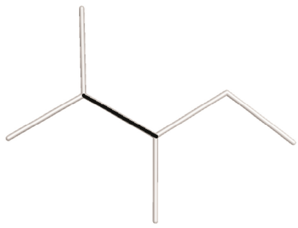
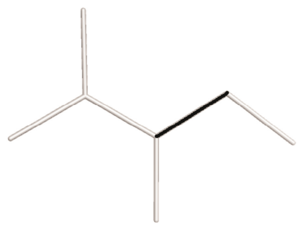
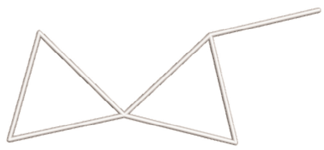
1		$CJ_e(x; i<j) = 4x^3 + 6x^6 + 4x^9$; $CJ_e'(1) = 84$
2		$CJ_e(x; i>j) = 4x^3 + 6x^6 + 4x^9$; $CJ_e'(1) = 84$
3	Global polynomial CJ $CJ_e(x) = 8x^3 + 12x^6 + 8x^9$; $CJ(1) = 28 = 2e$; $CJ'(1) = 168 = \mathrm{v} \times \mathrm{e}$ $CJ_p(x) = 16x^2 + 20x^3 + 24x^4 + 24x^5 + 16x^6 + 12x^7 + 12x^8 + 8x^9$; $CJ_p'(1) = 656$ $PI_v(x) = 14x^{12}$; $PI_v(1) = 14 = \mathrm{e}$; $PI_v'(1) = 168 = \mathrm{v} \times \mathrm{e}$	

Table 3. Counting polynomials in trees (bipartite graphs)

	Graph G10	Polynomial
1		$\mathrm{CJ_e}(x) = (4x^1 + 4x^6) + (x^2 + x^5) + (x^3 + x^4)$ $\mathrm{CJ_e}(1) = 2\mathrm{e} = 2\lvert E(G)\rvert = 12;\ \mathrm{v} = \lvert V(G)\rvert = 7$ $\mathrm{CJ_e}'(1) = 42 = \mathrm{ev}$ $\mathrm{CJ_e}''(1) = 160$
2		$(4x^1 + 4x^6)$
3		$(x^3 + x^4)$
4		$(x^2 + x^5)$
5	 L(G10)	$\mathrm{CJ}(x) = 7x^1 + 2x^2 + 2x^3 + 2x^4 + 1x^5$ $\mathrm{CJ}(1) = 14$ $\mathrm{CJ}'(1) = 30$ $\mathrm{PI_e}(G10) = 6\mathrm{x}^5$ $\mathrm{PI_e}'(1) = 30$

global polynomial, as shown in Table 1, entry 3, left hand column, and referred hereafter as the Cluj-edge $\mathrm{CJ_e}$ polynomial, or simply denoted CJ. Correspondingly, the Cluj-path $\mathrm{CJ_p}$ polynomial is presented in the right hand column, entry 3, Table 1. An example for the case of bipartite graphs is given in Table 2.

A particular case of bipartite graphs are the tree graphs (*e.g.*, G10, Table 3). It can be seen that the terms of CJ polynomial represent (connected) fragments of *k*-vertices: the figures in Table 3 illustrate the twin fragments, at the ends of each edge type (left hand column) and the corresponding associate terms in polynomial (right hand column).

In trees, we have the following

Theorem 1. *The sum of all path-counted vertex proximities in G is twice the sum of all distances in G or twice the Wiener index W:* $p_p = CJ'_p(1) = 2W$.

Proof. The column sums in the $\mathbf{UCJ}_\mathrm{p}$ matrix equals the column sums in the matrix of distances while the row sums in this matrix are identical to those in the Wiener matrix.[18,19] Half of the sum of entries in these matrices equals the sum of all distances in a tree graph, or its Wiener index.[30] Since the first derivative of $\mathrm{CJ_p}$ polynomial is just the sum of all entries in $\mathbf{UCJ}_\mathrm{p}$ matrix, the theorem is thus demonstrated.

Table 4. Formulas for counting CJ_e and PI_v polynomials in several classes of bipartite graphs

Phenylenes PHE_h; h = number of hexagons in molecule
$CJ_e(PHE_h, x) = 4 \cdot \sum_{k=1}^{h-1} x^{6k} + 8 \cdot \sum_{k=0}^{h-1} x^{6k+3} + 4h \cdot x^{3h}$ $CJ_e'(PHE_h, 1) = PI_v'(PHE_h, 1) = v \cdot e = 6h(8h-2)$ $CJ_e''(PHE_h, 1) = 3h(32h^2 - 33h + 11)$
$v(PHE_h) = 6h$; $e(PHE_h) = 8h - 2$
$PI_v(PHE_h, x) = e \cdot x^v = (8h-2)x^{6h}$ $PI_v''(PHE_h, 1) = e \cdot v \cdot (v-1) = 12h(6h-1)(4h-1)$

Coronenes COR_r; r = number of hexagon rows around the central hexagon
$CJ_e(COR_r, x) = \sum_{k=0}^{r} 6(r+k+2) \cdot x^{(k+1)(2r+k+3)} + \sum_{k=0}^{r-1} 6(r+k+2) \cdot x^{6(r+1)^2 - (k+1)(2r+k+3)}$ $CJ_e'(COR_r, 1) = PI_v'(COR_r, 1) = e \cdot v = 18(r+1)^3(3r+2)$ $CJ_e''(COR_r, 1) = 3(r+1)^2(72r^4 + 252r^3 + 307r^2 + 152r + 24)$
$v = 6(r+1)^2$; $e = 3(r+1)(3r+2)$
$PI_v(COR_r, x) = e \cdot x^v = 3(r+1)(3r+2)x^{6(r+1)^2}$ $PI_v''(COR_r, 1) = e \cdot v \cdot (v-1) = 18(3r+2)(6r^2 + 12r + 5)(r+1)^3$

Cubic lattice ($C_{k,k,k}$)
$CJ_e(C_{k,k,k}, x) = 6(k+1)^2 \sum_{i=1}^{k} x^{i(k+1)^2}$ $CJ_e'(C_{k,k,k}, 1) = PI_v'(C_{k,k,k}, 1) = e \cdot v = 3k(k+1)^2(k+1)^3$ $CJ_e''(C_{k,k,k}, 1) = k(k+1)^5(2k^3 + 5k^2 + 4k - 2)$
$v(C_{k,k,k}) = (k+1)^3$; $e(C_{k,k,k}) = 3k(k+1)^2$
$PI_v(C_{k,k,k}, x) = ex^v = 3k(k+1)^2 x^{(k+1)^3}$ $PI_v''(C_{k,k,k}, 1) = e \cdot v \cdot (v-1) = 3k^2(k^2 + 3k + 3)(k+1)^5$

3. VERTEX PI POLYNOMIAL

The vertex PI_v index of a graph is calculated by

$$PI_v = \sum_{e=uv} n(u,v) + n(v,u) = |V| \cdot |E| - \sum_{e=uv} m(u,v) \quad (7)$$

where n(u,v) is the number of vertices lying closer to the vertex u than the vertex v, and m(u,v) is the number of vertices that are at equal distance from the vertices u and v.[31–38] The vertex PI polynomial is defined as

$$PI_v(x) = \sum_{e \in E(G)} x^{n(u,v)+n(v,u)} = \sum_k m(k) \cdot x^k$$

Obviously $PI_v(1) = |E|$, while the first derivative of the vertex *PI* polynomial is equal to the vertex PI index, $PI_v'(1) = PI_v$.

It can be easily found that for any edge $e = (i,j)$ holds $CJ(i,j) = n(i,j)$. The sum of all entries in CJ_e matrix is equal to the sum of all $n(i, j)$ for adjacent vertices i and j, and therefore, we have the following

Theorem 2. *For any graph G, the equality* $CJ_e = PI_v$ *holds.*

Proof comes out from the observation that PI_v always counts the sum of contributions of both ends of any edge while CJ counts them separately; next, by associating them, we obtain the pair-wise sums of PI_v terms, as illustrated for the graph G10, in Table 1, entry 4 and Table 3, entries 1 to 4.

In bipartite graphs there are no equidistant vertices with respect to any two adjacent vertices, thus we have the following

Corollary 3. *In bipartite graphs, the equalities* $CJ_e = PI_v = |V| \cdot |E|$ *and* $PI_v(x) = |E| \cdot x^{|V|}$ *hold.*

4. SOME MORE REMARKS

The index PI_v calculated on the line graph (*i.e.*, the graph derived by putting a point on each edge/line of *G* and joining two such points if the parent edges were sharing an angle in *G*) equals the edge-version[31–33] PI_e, at least in case *G* is a tree, as shown in Table 3, entry 5.

Among the properties of counting polynomials, the value in $x = 1$ and the first derivative in $x = 1$ are the most important. In the case of the CJ_e polynomial, the value in $x = 1$, $CJ_e(1) = 2e$. It is evident, since every edge is visited twice. In the case of PI_v polynomial $PI_v(1) = e$, because at any edge in the graph, the local contributions are summed for the both ends at once. Their first derivatives provide indices, both counting non-equidistant vertices in the graph, both using summation at the operational stage; PI_v uses the associative property of this operation in reducing at about half the number of terms, in general graphs or at a single term, in case of bipartite ones (Table 2, entry 3). Their second derivative is, however, different (see tables above).

Recall that Szeged index[39–41] SZ, a topological index related to the Wiener index, also does not count the equidistant vertices in the graph. The difference between SZ and PI_v is the first index is calculated by multiplication of the local contributions while the second one by summation. Note that the multiplicative CJ index CJ_e equals the value of SZ index in any graph, while the corresponding indices calculated on path are always different.

Formulas for calculating CJ_e and PI_v polynomials in phenylenes, coronenes and cubic lattice are given in Table 4. Applications of these descriptors were described elsewhere.[25–27]

5. CONCLUSIONS

Cluj polynomials have been defined to count the proximities, as connected subgraphs/fragments, of the endpoints of any edge (CJ_e) or any path (CJ_p) in a graph. Their terms can be calculated either by summing the entries in the previously described unsymmetric Cluj matrices or by the well-known edge-cutting procedure.

The more recently proposed PI_v polynomial has proved to give identical value of its first derivative (in $x = 1$) as the CJ_e polynomial; it uses the associative property of summation of the local contributions, in fact identically defined as those of CJ_e polynomial. The second derivative is different for the two polynomials.

Analytical formulas for calculating these polynomials in several classes of bipartite graphs were developed.

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SAŽETAK

Cluj CJ i PIv polinomi

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U radu je predstavljena paralela između prebrojavajućih polinoma CJ(x) i PIv(x), koji su definirani od strane istraživačkih grupa profesora Diudea (Rumunjska) i Ashrafi (Iran), respektivno. Oba polinoma prebrojavaju neekvidistantne čvorove u odnosu na sve bridove grafa; razlika se javlja u operativnom dijelu, što je i demonstrirano u radu. Prvi izvodi u točki $x = 1$ imaju istu vrijednost; dok su drugi izvodi različiti. Prikazane su analitičke relacije za računavanje ovih polinoma i odgovarajućih brojevnih deskriptora na nekim klasama grafova.