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CLUJ CJ POLYNOMIAL AND INDICES IN A DENDRITIC MOLECULAR GRAPH

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ABSTRACT. The Cluj polynomials $CJ_e(x)$ and indices are calculable by either summation $CJ_eS(x)$ or multiplication $CJ_eP(x)$ of the sets of non-equidistant vertices related to the endpoints of any edge $e=(u,v)$ in the graph. A third polynomial, the (vertex) $PIv(x)$, is related to CJ_eS. In this paper, a procedure based on orthogonal cuts is used to derive the three above polynomials and indices in the molecular graph of a dendrimer.

Keywords: *dendrimer, molecular graph, Cluj polynomial, Cluj index*

INTRODUCTION

Cluj matrices and indices have been proposed by Diudea twelve years ago. A Cluj fragment [1-4] $CJ_{i,j,p}$ 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 $D_{(G-p)}$:

$$CJ_{i,j,p} = \{v \mid v \in V(G);\, D_{(G-p)}(i,v) < D_{(G-p)}(j,v)\} \tag{1}$$

In trees, $CJ_{i,j,p}$ denotes sets of (connected) vertices *v* joined with *j* by paths *p* going through *i*. The path *p*(*i*,*j*) is characterized by a single endpoint, which is sufficient to calculate the unsymmetric matrix UCJ.

In graphs containing rings, the choice of the appropriate path is quite difficult, thus that path which provides the fragment of maximum cardinality is considered:

$$[\mathbf{UCJ}]_{\boldsymbol{i,j}} = \max_{p} \left| CJ_{i,j,p} \right| \tag{2}$$

When 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[5]

$$SM_p = UM \bullet (UM)^T \tag{3}$$

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

$$SM_e = SM_p \bullet A \tag{4}$$

The basic properties and applications of the above matrices and derived descriptors have been presented elsewhere [6-11]. Notice that the Cluj indices, previously used in correlating studies published by TOPO GROUP Cluj, were calculated on the symmetric matrices, thus involving a multiplicative operation. Also, the symbol CJ (Cluj) is used here for the previously denoted CF (Cluj fragmental) matrices and indices.

Our interest is here related to the unsymmetric matrix defined on distances and calculated on edges $\mathbf{UCJ_e}$

$$UCJ_e = UCJ_p \bullet A \tag{5}$$

which provides the coefficients of the Cluj polynomials [12,13] (see below).

CLUJ POLYNOMIALS

A counting polynomial can be written in a general form as:

$$P(x) = \sum_k m(k) \cdot x^k \tag{6}$$

It counts a graphical property, partitioned in *m* sets of extent *k*, of which re-composition will return the global property. As anticipated in introduction, the Cluj polynomials count the vertex proximity of the both ends of an edge *e*=(*u*,*v*) in *G*; there are Cluj-edge polynomials, marked by a subscript *e* (edge), to be distinguished to the Cluj-path polynomials (marked by a subscript *p*), defined on the concept of distance DI or detour DE in the graph [2,5].

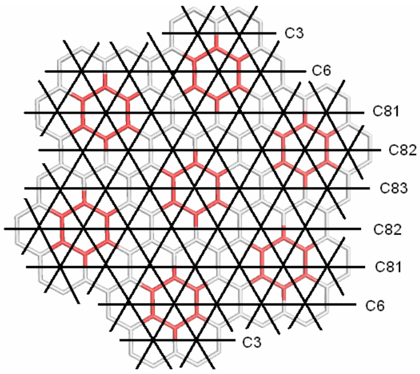
The coefficients *m*(*k*) of eq. (6) can be calculated from the entries of unsymmetric Cluj matrices, as provided by the TOPOCLUJ software program [14] or other simple routines. In bipartite graphs, a simpler procedure enabling the estimation of polynomial coefficients is based on orthogonal edge-cutting. The theoretical background of the edge-cutting procedure is as follows.

A graph *G* is a *partial cube* if it is embeddable in the *n*-cube Q_n, which is the regular graph whose vertices are all binary strings of length *n*, two strings being adjacent if they differ in exactly one position.[15] The distance function in the *n*-cube is the Hamming distance. A hypercube can also be expressed as the Cartesian product: $Q_n = W_{i=1}^{n} K_2$.

For any edge *e*=(*u*,*v*) of a connected graph *G* let n_{uv} denote the set of vertices lying closer to *u* than to *v*: $n_{uv} = \{w \in V(G) \mid d(w,u) < d(w,v)\}$. It follows that $n_{uv} = \{w \in V(G) \mid d(w,v) = d(w,u)+1\}$. The sets (and subgraphs) induced by these vertices, n_{uv} and n_{vu}, are called *semicubes* of *G*; the semicubes are called *opposite semicubes* and are disjoint [16,17].

A graph *G* is bipartite if and only if, for any edge of *G*, the opposite semicubes define a partition of *G*: $n_{uv} + n_{vu} = v = |V(G)|$. These semicubes are just the vertex proximities (see above) of (the endpoints of) edge *e*=(*u*,*v*), which the Cluj polynomials count.

In bipartite graphs, the opposite semicubes can be estimated by an orthogonal edge-cutting procedure, as shown in Figure 1. The set of edges intersected by an orthogonal line is called an (orthogonal) cut *Cn* and consists of (topologically) parallel edges; the associate number counts the intersections with the orthogonal line. In the right hand part of Figure 1, there are three numbers in the front of brackets, with the meaning: (i) symmetry; (ii) occurrence (in the whole structure) and (iii) *n*, the number of edges cut-off by an ortogonal line. The product of the above three numbers will give the coefficients of the Cluj polynomials. The exponents in each bracket represent the number of points lying to the left and to the right of the corresponding ortogonal line segment. A similar procedure has been used by Gutman and Klavžar to calculate the Szeged index of polyhex graphs [18].



$CJ_e\,S(x) = 3{\cdot}2{\cdot}3(x^{5}+x^{121}) + 3{\cdot}2{\cdot}6(x^{16}+x^{110}) + 3{\cdot}2{\cdot}8(x^{31}+x^{95}) + 3{\cdot}2{\cdot}8(x^{47}+x^{79}) + 3{\cdot}1{\cdot}8(x^{63}+x^{63})$

$CJ_e\,S'(1) = 21924$; $CJ_e\,S''(1) = 1762320$

$PI_v(x) = 3{\cdot}2{\cdot}3(x^{5+121}) + 3{\cdot}2{\cdot}6(x^{16+110}) + 3{\cdot}2{\cdot}8(x^{31+95}) + 3{\cdot}2{\cdot}8(x^{47+79}) + 3{\cdot}1{\cdot}8(x^{63+63})$

$PI_v'(1) = 21924$; $PI_v''(1) = 2740500$

$CJ_e\,P(x) = 3{\cdot}2{\cdot}3(x^{5\cdot121}) + 3{\cdot}2{\cdot}6(x^{16\cdot110}) + 3{\cdot}2{\cdot}8(x^{31\cdot95}) + 3{\cdot}2{\cdot}8(x^{47\cdot79}) + 3{\cdot}1{\cdot}8(x^{63\cdot63})$

$CJ_e\,P'(1) = 489090$

Figure 1. Edge-cutting procedure in the calculus of *CJ* polynomials of a bipartite graph

Three different counting polynomials can be defined on the vertex proximities/semicubes in bipartite graphs, which differ by the operation used in re-composing the edge contributions:

(i) *Summation*, and the polynomial is called *Cluj-Sum* (Diudea *et al*. [12,13,19,20]) and symbolized CJ_eS:

$$CJ_eS(x) = \sum\nolimits_e \left(x^{n_e} + x^{v-n_e} \right) \tag{7}$$

(ii) *Pair-wise summation*, with the polynomial called (vertex) Padmakar-Ivan [21,22] (Ashrafi [23-26]) and symbolized PI_v:

$$PI_v(x) = \sum\nolimits_e x^{n_e + (v-n_e)} \tag{8}$$

(iii) *Product*, while the polynomial is called *Cluj-Prod* and symbolized CJ_eP:

$$CJ_eP(x) = \sum\nolimits_e x^{n_e(v-n_e)} \tag{9}$$

Because the opposite semicubes define a partition of vertices in a bipartite graph, it is easily to identify the two semicubes in the above formulas: $n_{uv}=n_e$ and $n_{vu}=v$-n_e, or vice-versa.

The first derivative (in x=1) of a (graph) counting polynomial provides single numers, often called topological indices.

It is not difficult to see that the first derivative (in x=1) of the first two polynomials gives one and the same value, however, their second derivative is different (see Figure 1) and the following relations hold in any graph [20]:

$$CJ_eS'(1) = PI_v{}'(1)\,;\; CJ_eS''(1) \neq PI_v{}''(1) \tag{10}$$

The number of terms, $CJ_e(1)=2e$, is twice the number given by $PI_v(1)$ because, in the last case, the endpoint contributions are summed together for any edge in G (see (7) and (8)).

Clearly, the third polynomial is more different; notice that Cluj-Prod $CJ_eP(x)$ is precisely the (vertex) Szeged polynomial $Sz_v(x)$, defined by Ashrafi *et al*. [24-26] This comes out from the relations between the basic Cluj (Diudea [2,5]) and Szeged (Gutman [5,27]) indices:

$$CJ_eP'(1) = CJ_eDI(G) = Sz(G) = Sz_v{}'(1) \tag{11}$$

Recall the definition of the vertex PI_v index:

$$PI_v(G) = PI_v{}'(1) = \sum_{e=uv} n_{u,v} + n_{v,u} = |V|\cdot|E| - \sum_{e=uv} m_{u,v} \tag{12}$$

where $n_{u,v}$, $n_{v,u}$ count the non-equidistant vertices *vs*. the endpoints of e=(u,v) while $m(u,v)$ is the number of vertices lying at equal distance from the vertices u and v. All the discussed polynomials and indices do not count the equidistant vertices, an idea introduced in Chemical Graph Theory by Gutman. In bipartite graphs, since there are no equidistant vertices vs any edge, the last term in (12) will disappear. The value of $PI_v(G)$ is thus maximal in bipartite graphs, among all graphs on the same number of vertices; the result of (12) can be used as a criterion for checking the "bipatity" of a graph.

APPLICATION

The three above polynomials and their indices are calculated on a dendritic molecular graph, a (bipartite) periodic structure with the repeat unit v_0=8 atoms, taken here both as the root and branching nodes in the design of the dendron (Figure 2, see also refs. [27-30]).

Formulas collect the contributions of the *Root*, the internal (*Int*) and external (Ext) parts of the structure but close formulas to calculate first derivative (in x=1) of polynomials were derived for the whole molecular graph. Formulas for calculating the number of vertices, in the whole wedge or in local ones, and the number of edges are also given. Examples, at the bottom of Tables 1 and 2, will enable the reader to verify the presented formulas.

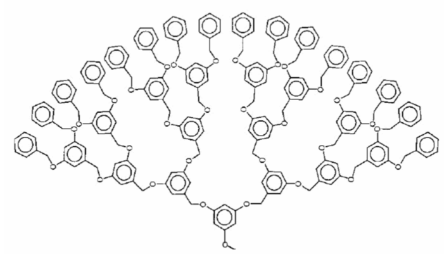


Figure 2. A dendritic wedge, of generation r=4; v=248; e=278.

Table 1. Formulas for counting CJ_eS and PI_v polynomials in a dendritic D wedge graph

$$CJ_eS(D,x) = CJ_eS(Root) + CJ_eS(Int) + CJ_eS(Ext)$$

$$CJ_eS(Root) = (x^1 + x^{v-1}) + (x^2 + x^{v-2}) + 1\cdot 2\cdot (x^5 + x^{v-5}) + 2\cdot 2\cdot (x^{v/2-1} + x^{v/2+1})$$

$$CJ_eS(Int) = \sum_{d=1}^{r-1}\{2^{r-d}\cdot 2\cdot 2\cdot [x^{v_d+3} + x^{v-(v_d+3)}] + 2^{r-(d+1)}\cdot 2\cdot 2\cdot [x^{v_{d+1}-5} + x^{v-(v_{d+1}-5)}] + 2^{r-(d+1)}\cdot 2\cdot 1\cdot \{[x^{v_{d+1}-2} + x^{v-(v_{d+1}-2)}] + [x^{v_{d+1}-1} + x^{v-(v_{d+1}-1)}] + [x^{v_{d+1}} + x^{v-v_{d+1}}]\}\}$$

$$CJ_eS(Ext) = 2^r\cdot 3\cdot 2\cdot (x^3 + x^{v-3}) + 2^r\cdot 1\cdot 1\cdot \{[x^{v_0-2} + x^{v-(v_0-2)}] + [x^{v_0-1} + x^{v-(v_0-1)}] + [x^{v_0} + x^{v-v_0}]\}$$

$$CJ_e{}'S(1) = CJ_eS(D) = v\cdot (8 + \sum_{d=1}^{r-1} 18\cdot 2^{r-(d+1)} + 9\cdot 2^r) = v\cdot (18\cdot 2^r - 10) = v\cdot e$$

$$v = v(D,r) = 2^3(2^{r+1}-1);\; v_d = 2^3(2^d-1);\; d = 1,2,..\; e(D) = 18\cdot 2^r - 10$$

Example:
$v(r=3)=120$; $e(r=3)=134$; $v(r=4)=248$; $e(r=4)=278$

$$PI_v(x) = e\cdot x^v = (18\cdot 2^r - 10)\cdot x^{2^3(2^{r+1}-1)};\quad PI_v{}'(1) = v\cdot e$$

Example:

$CJ_eS(x,r=3)=(1x^1+1x^{119})+(1x^2+1x^{118})+(48x^3+48x^{117})+(2x^5+2x^{115})+(8x^6+8x^{114})+(8x^7+8x^{113})+(8x^8+8x^{112})+(16x^{11}+16x^{109})+(8x^{19}+8x^{101})+(4x^{22}+4x^{98})+(4x^{23}+4x^{97})+(4x^{24}+4x^{96})+(8x^{27}+8x^{93})+(4x^{51}+4x^{69})+(2x^{54}+2x^{66})+(2x^{55}+2x^{65})+(2x^{56}+2x^{64})+(4x^{59}+4x^{61})$

$CJ_eS'(1,r=3)=16080$; $CJ_eS'(1,r=4)=68944$.

Table 2. Formulas for counting CJ_eP polynomial in a dendritic D wedge graph

$$CJ_eP(D,x) = CJ_eP(Root) + CJ_eP(Int) + CJ_eP(Ext)$$

$$CJ_eP(G) = \sum\nolimits_e \left(x^{n_e(v-n_e)}\right)$$

$$CJ_eP(Root) = x^{1(v-1)} + x^{2(v-2)} + 1\cdot 2\cdot [x^{5(v-5)}] + 2\cdot 2\cdot [x^{(v/2-1)(v/2+1)}]$$

$$CJ_eP(Int) = \sum_{d=1}^{r-1}\{2^{r-d}\cdot 2\cdot 2\cdot [x^{(v_d+3)(v-(v_d+3))}] + 2^{r-(d+1)}\cdot 2\cdot 2\cdot [x^{(v_{d+1}-5)(v-(v_{d+1}-5))}] + 2^{r-(d+1)}\cdot 2\cdot 1\cdot \{[x^{(v_{d+1}-2)(v-(v_{d+1}-2))}] + [x^{(v_{d+1}-1)(v-(v_{d+1}-1))}] + [x^{(v_{d+1})(v-v_{d+1})}]\}\}$$

$$CJ_eP(Ext) = 2^r\cdot 3\cdot 2\cdot (x^{3(v-3)}) + 2^r\cdot 1\cdot 1\cdot \{[x^{(v_0-2)(v-(v_0-2))}] + [x^{(v_0-1)(v-(v_0-1))}] + [x^{v_0(v-v_0)}]\}$$

$$CJ_e'P(1) = CJ_eP(D) = 3626 \cdot 2^r + 256 \cdot 2^{2r} - 3872 \cdot 4^r +$$
$$+1792 \cdot 4^r \cdot r + 1120 \cdot 2^r \cdot r + 99$$

Example:

$CJ_eP(x,r=3)=x^{119}+x^{236}+48x^{351}+2x^{575}+8x^{684}+8x^{791}+8x^{896}+16x^{1199}+8x^{1919}+4x^{2156}+4x^{2231}+4x^{2304}$ $+ 8x^{2511}+4x^{3519}+2x^{3564}+2x^{3575}+2x^{3584}+4x^{3599}$

$CJ_eP'(1,r=3)=168627$; $CJ_eP'(1,r=4)=1039107$.

CONCLUSIONS

Two Cluj polynomials $CJ_e(x)$ and indices, defined on vertex proximities/ semicubes, are calculable by either summation $CJ_eS(x)$ or multiplication $CJ_eP(x)$ of the sets of non-equidistant vertices related to the endpoints of any edge $e=(u,v)$ in the graph. A third polynomial, the (vertex) $PI_v(x)$, was shown to be related to the CJ_eS. A procedure based on orthogonal cuts, enabled us to derive the three above polynomials and indices in the molecular graph of a dendrimer. The procedure is applicable only in bipartite graphs.

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