

Subgraphs of Pair Vertices

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Topics

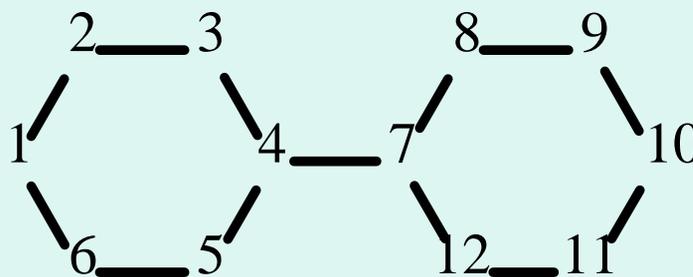
- **Definitions**
- **Square Matrices**
- **Counting Polynomials**
- **Subgraphs Properties**
- **Concluding Remarks**

Definitions

- $G = (V, E)$ graph \Leftrightarrow

- V : a set (vertices)

- E subset of $V \times V$ (edges)



- Notations: $V = V(G)$, $E = E(G)$
- G connected \Leftrightarrow is a path from one to any other vertex
- $V(\text{biphenyl}) = \{1, \dots, 12\}$
- $E(\text{biphenyl}) = \{(1,2), (2,3), (3,4), (4,5), (5,6), (1,6), (4,7), (7,8), (8,9), (9,10), (10,11), (11,12), (7,12)\}$

Definitions

- $P(G)$ – all paths from G
- $p(i,j)$ – a path from i to j
- $A(G)$ – adjacency matrix of G ;
- $D(G)$ – distance matrix of G ;
- $A(G)_{i,j} = 1$ if $(i,j) \in E(G)$, 0 otherwise
- $D(G)_{i,j} = |p(i,j)| < \infty$ for connected graphs

Definitions

- Gutman's Szeged (1994):
 - $SzF(G)_{i,j} = \{V(SzF(G)_{i,j}), E(SzF(G)_{i,j})\}$
 - $V(SzF(G)_{i,j}) = \{s \in V(G) \mid D(G)_{s,i} < D(G)_{s,j}\}$
 - $E(SzF(G)_{i,j}) = \{(s,t) \in E(G) \mid s,t \in V(SzF(G)_{i,j})\}$
- Diudea's Cluj (1997, 2001):
 - $CjF(G)_{i,j,p} = SzF(G_p)_{i,j}$
 - G_p is obtained from G by deleting the path p with exception of its endpoints

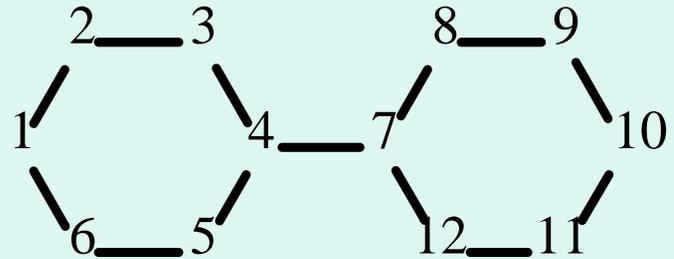
Definitions

- Minimal subgraph of G :
 - $MinF(G)_{i,j} = (\{i\}, \emptyset)$
- Maximal connected subgraph of G :
 - $VTmp(G)_{i,j} = \{s \in V(G) \mid s \neq j\}$
 - $ETmp(G)_{i,j} = \{(u,v) \in E(G) \mid u,v \neq j\}$
 - $V(MaxF(G)_{i,j}) = \{s \in VTmp(G)_{i,j} \mid D(VTmp(G)_{i,j})_{s,i} < \infty\}$
 - $E(MaxF(G)_{i,j}) = \{(s,t) \in E(G) \mid s,t \in V(MaxF(G)_{i,j})\}$
 - $MaxF(G)_{i,j} = (V(MaxF(G)_{i,j}), E(MaxF(G)_{i,j}))$

Square Matrices

- $[M]_{i,j} = |M(G)_{i,j}|$, where $M \in \{\text{MaxF}, \text{CMaxF}, \text{SZ}\}$
- $[CJ]_{i,j} = \max\{|CJF(G)_{i,j,p}|, p \in P(G)_{i,j}\}$

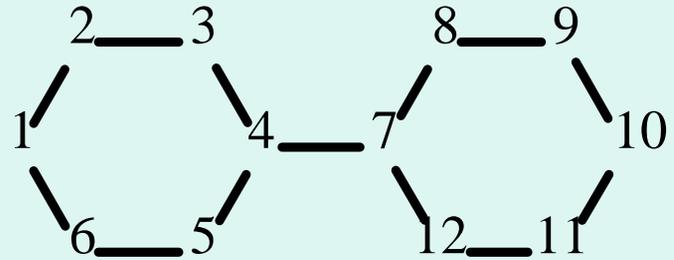
Square Matrices



MaxF	1	2	3	4	5	6	7	8	9	10	11	12	
1	0	11	11	5	11	11	6	11	11	11	11	11	110
2	11	0	11	5	11	11	6	11	11	11	11	11	110
3	11	11	0	5	11	11	6	11	11	11	11	11	110
4	11	11	11	0	11	11	6	11	11	11	11	11	116
5	11	11	11	5	0	11	6	11	11	11	11	11	110
6	11	11	11	5	11	0	6	11	11	11	11	11	110
7	11	11	11	6	11	11	0	11	11	11	11	11	116
8	11	11	11	6	11	11	5	0	11	11	11	11	110
9	11	11	11	6	11	11	5	11	0	11	11	11	110
10	11	11	11	6	11	11	5	11	11	0	11	11	110
11	11	11	11	6	11	11	5	11	11	11	0	11	110
12	11	11	11	6	11	11	5	11	11	11	11	0	110
	121	121	121	61	121	121	61	121	121	121	121	121	1332

$$MaxF(G, x) = 10x^5 + 12x^6 + 110x^{11}; D1|_{x=1} = 1332$$

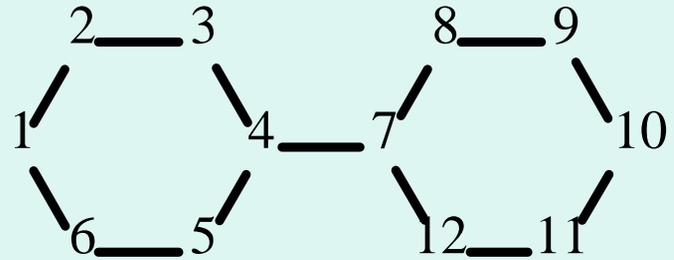
Square Matrices



CMaxF	1	2	3	4	5	6	7	8	9	10	11	12	
1	0	1	1	7	1	1	6	1	1	1	1	1	22
2	1	0	1	7	1	1	6	1	1	1	1	1	22
3	1	1	0	7	1	1	6	1	1	1	1	1	22
4	1	1	1	0	1	1	6	1	1	1	1	1	16
5	1	1	1	7	0	1	6	1	1	1	1	1	22
6	1	1	1	7	1	0	6	1	1	1	1	1	22
7	1	1	1	6	1	1	0	1	1	1	1	1	16
8	1	1	1	6	1	1	7	0	1	1	1	1	22
9	1	1	1	6	1	1	7	1	0	1	1	1	22
10	1	1	1	6	1	1	7	1	1	0	1	1	22
11	1	1	1	6	1	1	7	1	1	1	0	1	22
12	1	1	1	6	1	1	7	1	1	1	1	0	22
	11	11	11	71	11	11	71	11	11	11	11	11	252

$$CMaxF(G, x) = 110x + 12x^6 + 10x^7; D1|_{x=1} = 252$$

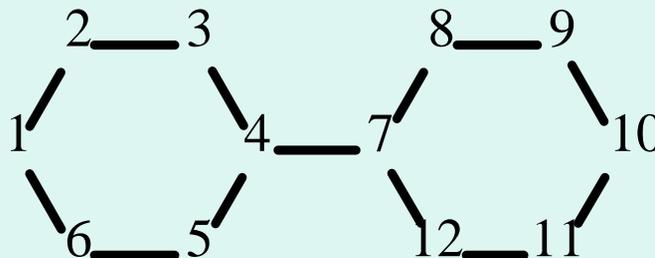
Square Matrices



SZ	1	2	3	4	5	6	7	8	9	10	11	12	
1	0	3	2	3	2	3	3	5	5	6	5	5	42
2	9	0	3	2	3	2	4	4	6	6	6	4	49
3	8	9	0	3	2	9	3	6	6	7	6	6	65
4	9	8	9	0	9	8	6	6	8	7	8	6	84
5	8	9	2	3	0	9	3	6	6	7	6	6	65
6	9	2	3	2	3	0	4	4	6	6	6	4	49
7	7	8	6	6	6	8	0	9	8	9	8	9	84
8	7	6	6	3	6	6	3	0	9	8	9	2	65
9	6	6	4	4	4	6	2	3	0	9	2	3	49
10	6	5	5	3	5	5	3	2	3	0	3	2	42
11	6	6	4	4	4	6	2	3	2	9	0	3	49
12	7	6	6	3	6	6	3	2	9	8	9	0	65
	82	68	50	36	50	68	36	50	68	82	68	50	708

$$SZ(G, x) = 16x^2 = 24x^3 + 12x^4 + 8x^5 + 36x^6 + 6x^7 + 12x^8 + 18x^9; D1|_{x=1} = 708$$

Square Matrices



CJ	1	2	3	4	5	6	7	8	9	10	11	12	
1	0	3	2	2	2	3	3	3	3	3	3	3	30
2	9	0	3	2	2	2	4	4	4	4	4	4	42
3	8	9	0	3	2	8	5	5	5	5	5	5	60
4	8	8	9	0	9	8	6	6	6	6	6	6	78
5	8	8	2	3	0	9	5	5	5	5	5	5	60
6	9	2	2	2	3	0	4	4	4	4	4	4	42
7	6	6	6	6	6	6	0	9	8	8	8	9	78
8	5	5	5	5	5	5	3	0	9	8	8	2	60
9	4	4	4	4	4	4	2	3	0	9	2	2	42
10	3	3	3	3	3	3	2	2	3	0	3	2	30
11	4	4	4	4	4	4	2	2	2	9	0	3	42
12	5	5	5	5	5	5	3	2	8	8	9	0	60
	69	57	45	39	45	57	39	45	57	69	57	45	624

$$CJ(G, x) = 22x^2 + 24x^3 + 24x^4 + 24x^5 + 12x^6 + 14x^8 + 12x^9; D1|_{x=1} = 624$$

Counting Polynomials

- a representation of a sequence of numbers, with the exponents showing the extent of partitions $p(G)$, of a graph property $P(G)$ while the coefficients are related to the occurrence of partitions of extent k

$$P(G, x) = \sum_k m(G, k) \cdot x^k$$

Counting Polynomials

$$\text{MaxF}(G, x) = 10x^5 + 12x^6 + 110x^{11}; D1|_{x=1} = 1332$$

$$\text{CMaxF}(G, x) = 110x + 12x^6 + 10x^7; D1|_{x=1} = 252$$

$$\text{SZ}(G, x) = 16x^2 + 24x^3 + 12x^4 + 8x^5 + 36x^6 + 6x^7 + 12x^8 + 18x^9; D1|_{x=1} = 708$$

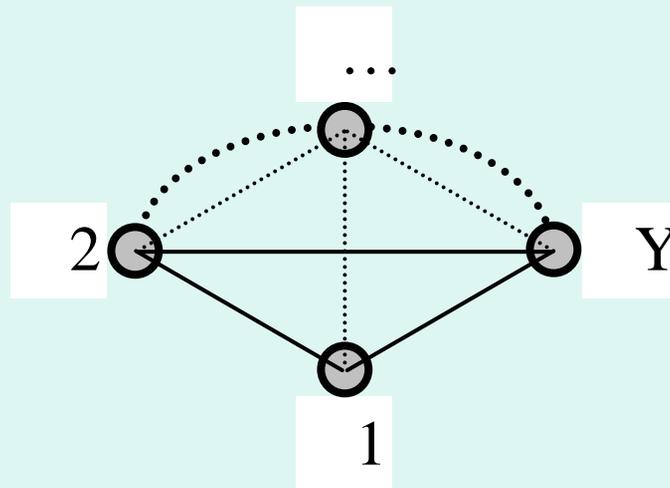
$$\text{CJ}(G, x) = 22x^2 + 24x^3 + 24x^4 + 24x^5 + 12x^6 + 14x^8 + 12x^9; D1|_{x=1} = 624$$



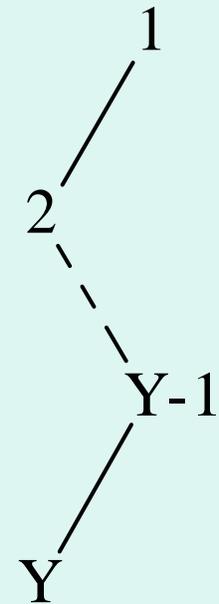
Counting Polynomials



Star, $S_{1,Y}$



Complete, K_Y



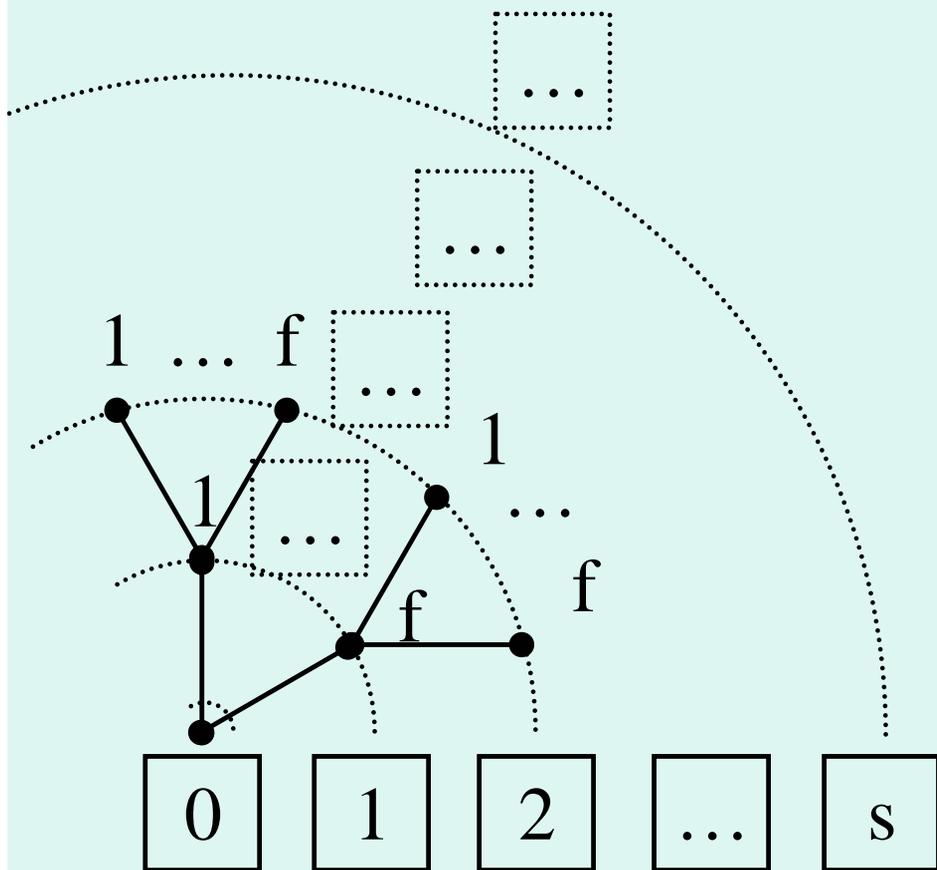
Path, P_Y

Counting Polynomials

G	Polynomial
1 Star $S_{1,n}$	$\text{MaxF}(G,x) = (n+1)x^0 + nx^1 + n^2x^n$ $\text{CMaxF}(G,x) = \text{SZ}(G,x) = \text{CJ}(G,x) = (n+1)x^0 + n^2x^1 + nx^n$
2 Path P_n	$\text{MaxF}(G,x) = nx^0 + 2\sum_{1 \leq k < n} kx^k$ $\text{CMaxF}(G,x) = \text{CJ}(G,x) = nx^0 + 2\sum_{1 \leq k < n} (n-k)x^k$ $\text{SZ}(G,x) = nx^0 + 4\sum_{1 \leq k \leq \binom{2n-1+(-1)^n}{4}} kx^k + 2\sum_{1 \leq k \leq \binom{2n-3+(-1)^n}{4}} (2k-1)x^{n+1-k}$
3 Complete K_n	$\text{MaxF}(G,x) = nx^0 + n(n-1)x^{n-1}$ $\text{CMaxF}(G,x) = \text{CJ}(G,x) = \text{SZ}(G,x) = nx^0 + n(n-1)x$



Counting Polynomials



Dendrimers $D_{f,s}$
Note: s letter in the dendrimers formula is the layer; on “0” layer there is 1 atom, on “1” layer there are f atoms (counting the number of atoms $n = f + 1$).

Counting Polynomials

G

Polynomial

Dendrimers*

$D_{f,s}$

$$\begin{aligned} \text{MaxF}(G,x) = & \frac{f(f-1)^s - 2}{f-2} x^0 + f \sum_{0 \leq k < s} (f-1)^{s-k-1} \frac{(f-1)^{k+1} - 1}{f-2} x^{\frac{(f-1)^{k+1} - 1}{f-2}} \\ & + f \sum_{0 \leq k < s} (f-1)^{s-k-1} \frac{f(f-1)^s - (f-1)^{k+1} - 1}{f-2} x^{\frac{f(f-1)^s - (f-1)^{k+1} - 1}{f-2}} \end{aligned}$$

$$\begin{aligned} \text{CMaxF}(G,x) = & \frac{f(f-1)^s - 2}{f-2} x^0 + f \sum_{0 \leq k < s} (f-1)^{s-k-1} \frac{f(f-1)^s - (f-1)^{k+1} - 1}{f-2} x^{\frac{(f-1)^{k+1} - 1}{f-2}} \\ & + f \sum_{0 \leq k < s} (f-1)^{s-k-1} \frac{(f-1)^{k+1} - 1}{f-2} x^{\frac{f(f-1)^s - (f-1)^{k+1} - 1}{f-2}} = \text{CJ}(G,x) \end{aligned}$$

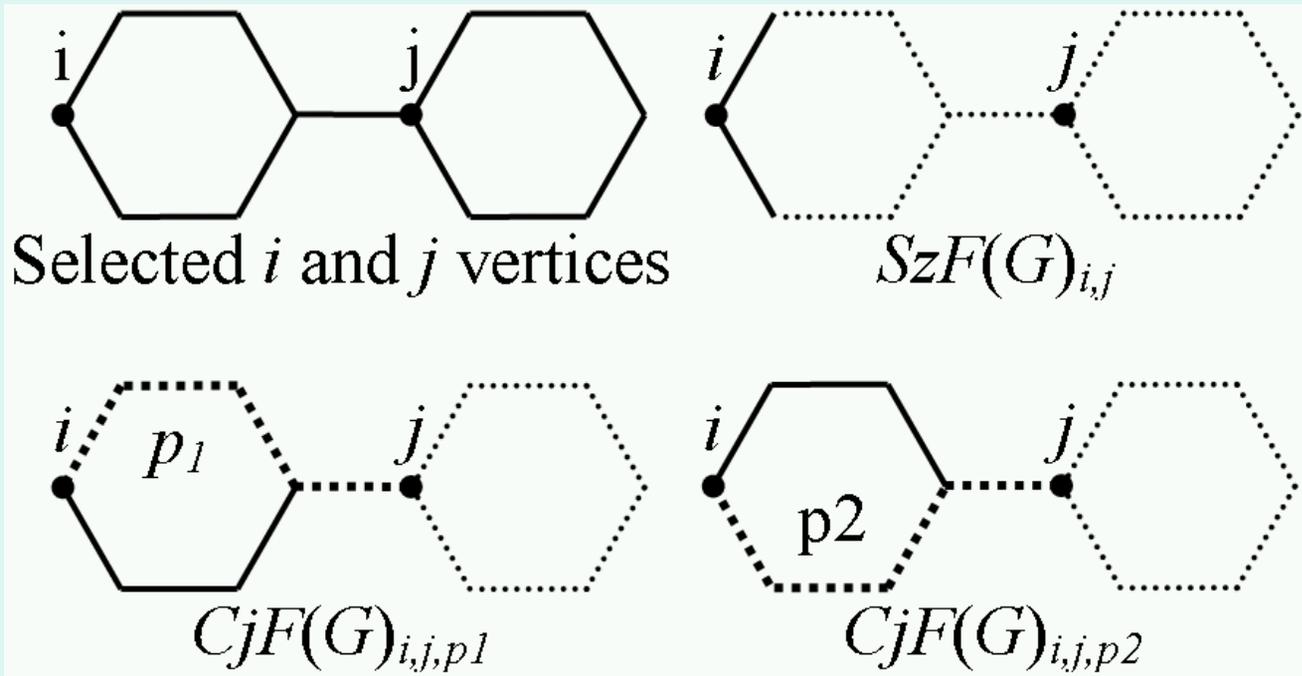
$$\begin{aligned} \text{SZ}(G,x) = & \frac{f(f-1)^s - 2}{f-2} x^0 \\ & + f \sum_{0 < k \leq s} \frac{(f-1)^{s-k}}{f-2} \left(((f-1)^{2k} - 1) x^{\frac{(f-1)^k - 1}{f-2}} + ((f-1)^{2k-1} - 1) x^{\frac{f(f-1)^s - (f-1)^k - 1}{f-2}} \right) \end{aligned}$$

Subgraphs Properties

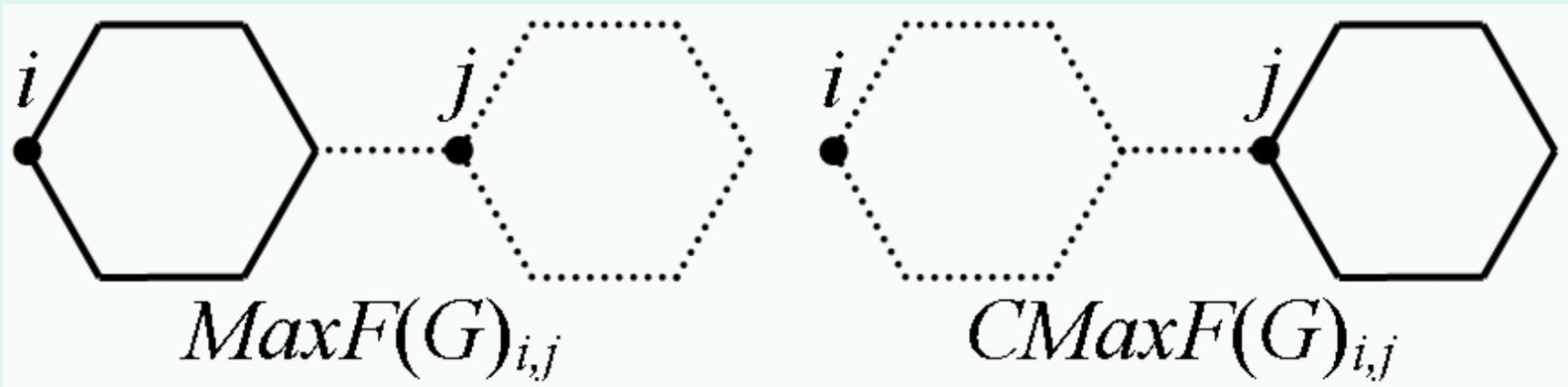
- Theorem 1

– In a not empty graph G , the following relations hold:

$$1 = n_{MinF} \leq n_{CjF}, n_{SZF} \leq n_{MaxF} \leq n_G; \text{ where } n_A = |A|$$

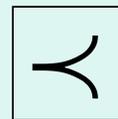


Subgraphs Properties



- Theorem 2

- $CMaxF(G)_{i,j} \prec G$

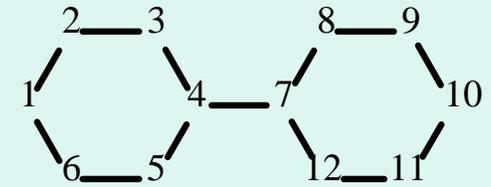


means connected subgraph

- Theorem 3

- $SzF(G)_{i,j} \prec CjF(G)_{i,j,p} \prec MaxF(G)_{i,j} \prec G$

Subgraphs Properties



MaxF	1	2	3	4	5	6	7	8	9	10	11	12	
1	0	11	11	5	11	11	6	11	11	11	11	11	110
2	11	0	11	5	11	11	6	11	11	11	11	11	110
3	11	11	0	5	11	11	6	11	11	11	11	11	110
4	11	11	11	0	11	11	6	11	11	11	11	11	116
5	11	11	11	5	0	11	6	11	11	11	11	11	110
6	11	11	11	5	11	0	6	11	11	11	11	11	110
7	11	11	11	6	11	11	0	11	11	11	11	11	116
8	11	11	11	6	11	11	5	0	11	11	11	11	110
9	11	11	11	6	11	11	5	11	0	11	11	11	110
10	11	11	11	6	11	11	5	11	11	0	11	11	110
11	11	11	11	6	11	11	5	11	11	11	0	11	110
12	11	11	11	6	11	11	5	11	11	11	11	0	110
	121	121	121	61	121	121	61	121	121	121	121	121	1332

$$MaxF(G, x) = 10x^5 + 12x^6 + 110x^{11}; D1|_{x=1} = 1332$$

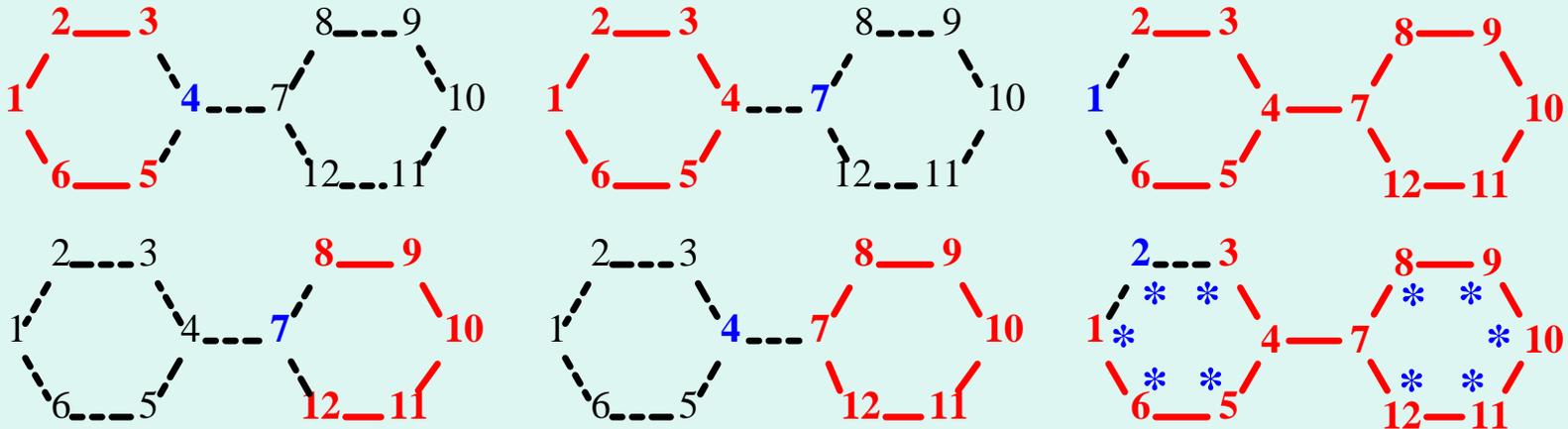
- $MaxF(G, x) = 2 \cdot 5 \cdot x^5 + 2 \cdot 6 \cdot x^6 + 10 \cdot 11 \cdot x^{11}$

Subgraphs Properties

$$\text{MaxF}(G,x) = 2 \cdot 5 \cdot x^5 + 2 \cdot 6 \cdot x^6 + 10 \cdot 11 \cdot x^{11}$$

- Theorem 4**

- *The number of occurrences of a given size subgraph, generated by MaxF criterion applied to a graph G, equals the number of vertices consisting the subgraph*



$\text{MaxF}(G)_{i,j}$ - red i, blue j

Subgraphs Properties

- Theorem 5

$$\begin{aligned} \sum n_{\text{MinF}} &= n_G \cdot (n_G - 1) \\ &\leq \sum n_{\text{CMaxF}} \leq \sum n_{\text{CJF}} \leq \sum n_{\text{SZF}} \leq \sum n_{\text{MaxF}} \leq \\ &n_G \cdot (n_G - 1)^2 = (n_G - 1) \sum n_{\text{MinF}} = \sum n_{\text{CMinF}} \end{aligned}$$

- CMinF:

- n_G choices of “i” selecting;
- $n_G - 1$ vertices (one out);
- $n_G - 1$ choices of “j” selecting;
- $n_G \cdot (n_G - 1) \cdot (n_G - 1)$

- MinF

- 1 vertex
- $n_G \cdot 1 \cdot (n_G - 1)$

Concluding Remarks

- (MinF) (\leq) (CMaxF) (\leq) (Szeged),(Cluj)
- (Szeged),(Cluj) (\leq) (MaxF) (\leq) (CMinF)
- Szeged, Cluj, MaxF, CMaxF counting polynomials:

$$\lim_{f \rightarrow 2} D_{f,s} = P_{2s+1}$$

Acknowledgments

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 - CEEEx/M2/C2/2005/ET/46
 - CEEEx/M2/C3/2006/ET/108
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- Prof. Dr. Ivan GUTMAN

Thank you for your attention!

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 - /molecular_topology/counting_polynomial/
 - /molecular_topology/vertex_cutting/



Book of Abstracts

20 Years Anniversary of Molecular Topology at Cluj

*Babes-Bolyai University
Faculty of Chemistry and Chemical Engineering*

*September 25 - 30, 2006
Cluj-Napoca, Romania*

Friday, 29 September

SESSION 10

Chairman: Adrian Beteringhe

9.00-9.30	<u>Lorentz Jäntschi</u> Subgraphs by Pairs of Vertices
9.30-10.00	<u>Maria Mracec</u> and Mircea Mracec 3D- and 2D-Electrotopological state indices and MTD descriptor in a QSAR study of psychotomimetic phenylalkylamines
10.00-10.30	Mircea V. Diudea, <u>Aniela E. Vizitiu</u> and Dušanka Janežič Cluj and related polynomials applied in QSPR studies

10.30-11.00 Coffee Break

SESSION 11

Chairman: Lorentz Jäntschi

11.00-11.30	<u>Urban Bren</u> and Matevž Bren Do all pieces make a whole?
11.30-12.00	<u>Costinel I. Lepădatu</u> Molecular descriptors for the “valence shell” of the molecule
12.00-12.30	<u>Janez Konc</u> and Dušanka Janežič A branch and bound algorithm for matching protein structures
12.30-13.00	<u>Adrian Beteringhe</u> , Petru Filip and Alexandru T. Balaban A new topological index (quadratic index Q)

13.00-15.00 Lunch

16.00-17.00 Closing Ceremony

Saturday, 30 September

Departures

Subgraphs by Pairs of Vertices

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Abstract

Subgraphs obtained by applying several fragmentation criteria are investigated. Two well known criteria (Szeged and Cluj),¹⁻⁵ and two new others are defined and characterized. An example is given for the discussed procedures. The matrix and polynomial representations of vertices consisting each type of subgraphs were also given. Analytical formulas for the polynomials of several classes of graphs are derived. The newly introduced subgraphs/fragments, called MaxF and CMaxF, appear to have interesting properties, which are demonstrated.

References

1. M.V. Diudea, I. Gutman and L. Jäntschi, *Molecular Topology*. Nova Science, Huntington, New York, 2001.
2. M. V. Diudea, *J. Chem. Inf. Comput. Sci.*, **1997**, *37*, 300-305.
3. M. V. Diudea, B. Parv, and I. Gutman, *J. Chem. Inf. Comput. Sci.*, **1997**, *37*, 1101-1108.
4. M. V. Diudea, G. Katona, I. Lukovits, and N. Trinajstić, *Croat. Chem. Acta*, **1998**, *71*, 459-471.
5. L. Jäntschi, G. Katona, and M. V. Diudea, *MATCH, Commun. Math. Comput. Chem.*, **2000**, *41*, 151-188.