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On Deletion–Contraction Polynomials for Polycyclic Chains*

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Abstract

A general calculating scheme of polynomials based on deletion-contraction operations is considered for polycyclic chains of polygons. Some chemically and combinatorially interesting polynomials could be embedded into this scheme. Explicit expressions are obtained for the Tutte and related polynomials. Polycyclic chains contain some classes of chemically relevant structures, in particular, molecular graphs of unbranched benzenoids hydrocarbons.

1 Introduction

Polynomial graph invariants have found interesting applications in organic chemistry and biology for characterization molecular graphs and DNA [1, 7, 17, 18, 20, 23, 28, 29]. These applications stimulate intensive studies of new and old well-known polynomial invariants. One of the famous invariants of this kind is the Tutte polynomial that gives interesting information about graph structure [3, 5, 14, 15]. In recent papers [13, 16], properties of the Tutte polynomials have been investigated for chemically relevant polycyclic graphs. In this paper we consider a general calculation scheme for a deletion-contraction polynomial invariant for classes of polycyclic graphs. A graph of such classes consists of

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n-gons in the plane connected with each other by an edge. Some of these classes include molecular graphs of polycyclic chemical compounds, in particular, molecular graphs of unbranched benzenoid hydrocarbons [8, 30]. The scheme is based on recurrent relations which are induced by two elementary graph operations: deletion and contraction of an edge. General explicit formulae for the polynomial will be presented (section 3). Several well-known polynomials are injected into this scheme with suitable coefficients. Among them are the Tutte polynomial (section 4), the Negami polynomial (section 5), the Yamada polynomial (section 6), the chromatic and the flow polynomials (sections 7 and 8).

2 Polycyclic graphs

All graphs considered in this paper are finite, undirected, connected, and may have loops and multiple edges. If G is a graph, $V(G)$ and $E(G)$ will denote its sets of vertices and edges, $|V(G)| = p$ and $|E(G)| = q$. A graph called the *chain of n-gons* consists of n-gons connected with each other by edges. Two arbitrary n-gons may have only a common edge, i.e., they are adjacent. Each n-gon is adjacent to no more than two other n-gons. There are no three n-gons which share a common edge but several n-gons may have a common vertex. Two *terminal* n-gons of a chain are adjacent to exactly one other n-gon.

Let U_k^n be the class of all chains with k copies of n-gons, where $k \geq 1$, $n \geq 2$. Graphs of U_k^n may be defined by recursion. We assume that $G \in U_0^n$ consists of a "degenerate" n-gon which is a single edge on two vertices for every $n \geq 2$. A graph $G \in U_k^n$, $k \geq 1$, $n \geq 2$, is obtained from some $H \in U_{k-1}^n$ by identifying an edge of a new n-gon with an edge of the terminal n-gons in H. A chain of U_k^n may be embedded into the plane such that all its interior faces will be n-gons. All polycyclic graphs of U_k^n for $2 \leq n \leq 6$ and $1 \leq k \leq 4$ are presented on Fig. 1. Results of analytical and computer enumerations of polycyclic chains of various classes have been reported in numerous articles (see, for example, [2, 4, 6, 9, 20, 21, 27]). The number of all graphs in U_k^n grows as n^k and may be presented by the following formula [6]:

$$|U_k^n| = \tfrac{1}{4}(n-3)^{k-2} \ + \ \tfrac{1}{8}[1-(-1)^n]\tbinom{2}{k} \ + \ \tfrac{1}{8}[1+(-1)^n]$$
$$+\tfrac{1}{4}(n-3)^{\lfloor \frac{k}{2} \rfloor -1}\left(\left\lfloor \tfrac{1}{2}(n-3)\right\rfloor [1-(-1)^k] + \tfrac{1}{2}[1-(-1)^n]\,[1+(-1)^k] + (-1)^n + 1\right).$$

Class U_k^n contains graphs which play an important role in the organic chemistry. For example, molecular graphs of unbranched catacondensed benzenoid hydrocarbons belong to U_k^6 [8, 30].

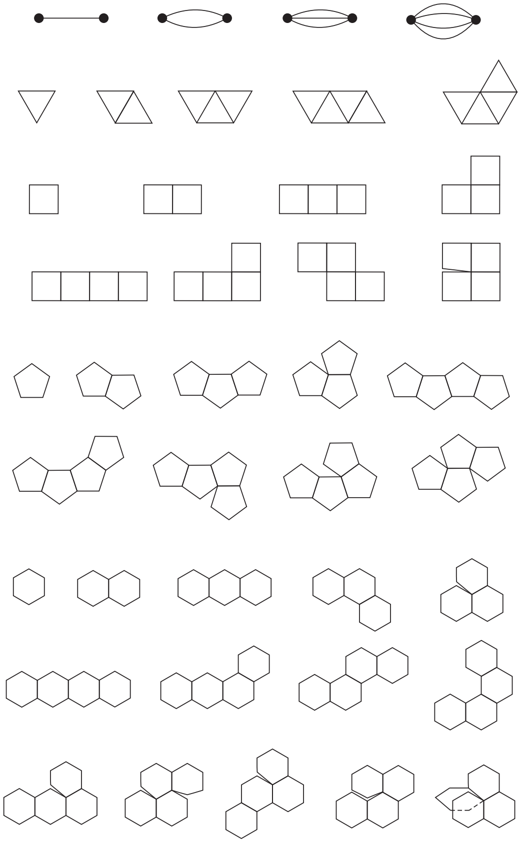

Figure 1: All chains of U_k^n with k n-gons for $n \leq 6$ and $k \leq 4$.

Two connected graphs G and H are said to be 2-*isomorphic* if G can be transformed into H by means of the following operation and its inverse: suppose G is obtained from the disjoint graphs G_1 and G_2 by identifying the vertices $u_1 \in V(G_1)$ with $u_2 \in V(G_2)$ and $v_1 \in V(G_1)$ with $v_2 \in V(G_2)$ (see Fig. 2).

Then graph H is obtained from G_1 and G_2 by identifying u_1 with v_2 and u_2 with v_1. This operation does not change the cycle structure of G and H [35]. An example of transformations of hexagonal chains is shown in Fig. 3.

It is easy to see that two arbitrary chains of U_k^n are 2-isomorphic.

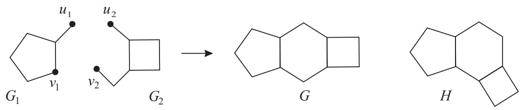

Figure 2: 2-isomorphic graphs G and H.

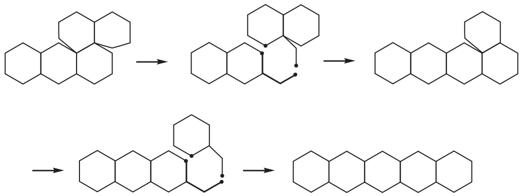

Figure 3: Transformations of 2-isomorphic hexagonal chains.

3 Function f defined by deletion-contraction operations

In this section, we define a function f by a recurrent calculating scheme with formal coefficients. Our aim is to derive an explicit formula of f for chains of n-gons. As a result, formulas for certain known polynomials can be obtained by specifying formal coefficients of the recurrent relations. In this section, we follow an approach developed in [11].

3.1 General scheme

As elementary operation of connected graphs, we consider the *deletion* and the *contraction* of edges. The resulting graph after deletion and contraction of an edge e will be denoted by $G - e$ and G/e, respectively. A graph G/e is obtained from G by deleting edge e and identifying its ends to a single vertex. An edge is called the *isthmus* if its removal increases the number of connected components in a graph. A graph function is called a 2-*invariant* if it assigns to 2-isomorphic graphs the same value.

Let f be a 2-invariant graph function with values from some ring R. We will assume that a function f satisfies the following conditions:

- if an edge e is not a loop or an isthmus, then

$$f(G) = A\, f(G/e) + B\, f(G - e), \tag{1}$$

where the coefficients A and B don't depend on the choice of e;

- if $H \cdot K$ is a union of two subgraphs H and K which have only a common vertex, then

$$f(H \cdot K) \,=\, C\, f(H)\, f(K), \tag{2}$$

where the coefficient C does not depend on the subgraphs H and K;

- if T_1 is a tree with a single edge on two vertices, then

$$f(T_1) \,=\, D; \tag{3}$$

- if L_1 is a single vertex with only loop, then

$$f(L_1) \,=\, E. \tag{4}$$

Applying the above properties of the function f, we may immediately calculate f for the simplest classes of graphs:

– if T_q is a connected tree with q edges, then

$$f(T_q) \,=\, C^{\,q-1}\, D^q;$$

– if L_q is a single vertex with q loops, then

$$f(L_q) \,=\, C^{\,q-1}\, E^{\,q};$$

– if M_q consists of two vertices joining by multiple q edges, then

$$f(M_q) \,=\, B^{\,q-1}\, D \,+\, A\, E\, \frac{B^{\,q-1} \,-\, (C\,E)^{\,q-1}}{B \,-\, C\,E},$$

– if C_q is a simple cycle with q edges, then

$$f(C_q) \,=\, A^{\,q-1}\, E \,+\, B\, D\, \frac{A^{\,q-1} \,-\, (C\,D)^{\,q-1}}{A \,-\, C\,D}. \tag{5}$$

Note that many polynomials satisfied conditions (1) – (4) belong to the so-called Tutte-Gröthendieck invariants [1, 14].

3.2 Formulas of f for polycyclic chains of U_k^n

Since the function f is 2-invariant, we shall denote the value $f(G)$ for an arbitrary graph $G \in U_k^n$ by f_k^n. Recall that the class U_0^n, $n \geq 2$, contains the degenerate n-gons. Then by (3)

$$f_0^n \,=\, f(T_1) \,=\, D\,.$$

Furthermore, the class U_1^n, $n \geq 2$, contains an n-gon only. By (5),

$$f_1^n = f(C_n) = A^{n-1} E + B D \frac{A^{n-1} - (C D)^{n-1}}{A - C D}. \tag{6}$$

Let $a_n = A^{n-2} C E + B \dfrac{A^{n-1} - (C D)^{n-1}}{A - C D}$ and $b_n = A^{n-2} B C^{n-1} D^{n-2} E$.

The following theorem gives a recurrent formula of the function f for chains of n-gons.

Theorem 1. [11] *For a chain with k n-gons, $n \geq 2$ and $k \geq 2$, we have*

$$f_k^n = a_n f_{k-1}^n - b_n f_{k-2}^n. \tag{7}$$

Form Theorem 1, the function f can be presented in the following form:

Corollary 1. [11] *For a chain with k n-gons, $n \geq 2$ and $k \geq 2$, we have:*

$$f_k^n = c_n^{k-1} f_1^n - d_n^{k-1} f_0^n,$$

where $\begin{pmatrix} c_n^k \\ d_n^k \end{pmatrix} = \begin{pmatrix} a_n & -1 \\ b_n & 0 \end{pmatrix}^{k-1} \begin{pmatrix} a_n \\ b_n \end{pmatrix}.$

The following formula can be obtained by standard methods from Theorem 1.

Corollary 2. *For a chain with k n-gons of U_k^n, $n \geq 2$ and $k \geq 2$, we have*

$$f_k^n = \frac{w_1}{2}\left(\frac{a_n + \sqrt{a_n^2 - 4b_n}}{2}\right)^k - \frac{w_2}{2}\left(\frac{a_n - \sqrt{a_n^2 - 4b_n}}{2}\right)^k.$$

where $w_1 = \dfrac{2f_1^n - a_n f_0^n}{\sqrt{a_n^2 - 4b_n}} + f_0^n$ *and* $w_2 = \dfrac{2f_1^n - a_n f_0^n}{\sqrt{a_n^2 - 4b_n}} - f_0^n$.

3.3 Generating function

Corollaries 1-2 allow the deriving explicit expressions for polynomials of chains. Another way is using generating functions. Let us fix $n \geq 3$. The *generating function* of a sequence $\{f_k^n\}_{k=0}^{\infty}$ is a formal power series $F(z) = \sum_{k=0}^{\infty} f_k^n z^k$.

Theorem 2. *The generating function $F(z)$ can be written as*

$$F(z) = \frac{\lambda + (\mu - \alpha\lambda)z}{1 - \alpha z - \beta z^2},$$

where $\alpha = a_n$, $\beta = -b_n$, $\lambda = f_0^n$ and $\mu = f_1^n$.

Proof. According to Theorem 1, function f_k^n can be calculated by the recurrent formula

$$f_k^n = \alpha f_{k-1}^n + \beta f_{k-2}^n. \tag{8}$$

Multiplying both parts of (8) by z^k and taking sums for $k = 2, 3, \ldots$, we get

$$F(z) - f_1^n z - f_0^n = \alpha z (F(z) - f_0^n) + \beta z^2 F(z).$$

Using initial conditions $f_0^n = \lambda$ and $f_1^n = \mu$ we get

$$F(z) - \mu z - \lambda = \alpha z F(z) - \alpha z \lambda + \beta z^2 F(z),$$

that implies the result. ∎

Corollary 3. *The generating function $F(z)$ can be written as follows:*

$$F(z) = \frac{D + A^{n-2} E (A - C D) z}{1 - \left(B \dfrac{A^{n-1} - (C D)^{n-1}}{A - C D} + A^{n-2} C E\right) z + \left(A^{n-2} B C^{n-1} D^{n-2} E\right) z^2}.$$

Expanding function $F(z)$ in a Taylor series, we can calculate coefficients for the members of the series $F(z) = f_0^n + f_1^n z + f_2^n z^2 + f_3^n z^3 + \ldots$.

In the next sections, we present several polynomials that can be obtained from f with suitable coefficients A, B, C, D, and E (see Table 1).

Table 1: Coefficients of recurrent expressions for polynomials.

Name	A	B	C	D	E
Tutte polynomial $T(G; x, y)$	1	1	1	x	y
Negami polynomial $N(G; t, x, y)$	x	y	$1/t$	$t(x + ty)$	$t(x + y)$
Yamada polynomial $h(G; x, y)$	1	$-1/x$	$1/x$	0	$xy - 1$
Chromatic polynomial $P(G; \lambda)$	-1	1	$1/\lambda$	$\lambda(\lambda - 1)$	0
Flow polynomial $F(G; \lambda)$	1	-1	1	0	$\lambda - 1$

4 Tutte polynomial

In this section, we apply properties of function f for calculating the Tutte polynomial of polycyclic chains. An arbitrary chain of U_k^n will be denoted by G_k^n.

4.1 General expressions

The Tutte polynomial $T(G;x,y)$ of a graph G is a 2-invariant function which was introduced as a two variable generalization of the chromatic polynomial [31]. It can be defined by the following equality:

$$T(G;x,y) = \sum_{Y\subset E(G)} (x-1)^{\omega(G-Y)-\omega(G)}(y-1)^{\beta(G-Y)},$$

where the summation goes over all edge subsets Y of $E(G)$, $\omega(G)$ is the number of connected components in G, and $\beta(G)$ is the cyclomatic number of a graph G with p vertices and q edges: $\beta(G) = q(G) - p(G) + \omega(G)$.

The Tutte polynomial is one of the important and useful invariants of a graph. It allows the extraction information on graph structure, e.g., the number of spanning trees, the number of connected subgraphs, the number of acyclic orientations, etc. It has found interesting applications in enumerative combinatorics, knot theory, statistical physics and computer science [3, 5, 14, 15, 34].

It is well known that the Tutte polynomial $T(G;x,y)$ satisfies the following recursive relation for a graph G:

$$T(G;x,y) = T(G/e;x,y) + T(G-e;x,y),$$

where e is not a loop or an isthmus. Further, if subgraphs H and K have only a common vertex, then the equality

$$T(H\cdot K;x,y) = T(H;x,y)\,T(K;x,y)$$

holds. For graphs T_1 and L_1 the polynomial is equal to $T(T_1;x,y) = x$ and $T(L_1;x,y) = y$.

Note, that $T(G;x,y)$ coincide with the function f under the coefficients $A=1$, $B=1$, $C=1$, $D=x$, and $E=y$. In this case for other quantities from Theorem 2, we have $a_n = y + \dfrac{x^{n-1}-1}{x-1}$, $b_n = y\,x^{n-2}$, $f_0^n = x$, and $f_1^n = y + x\,\dfrac{x^{n-1}-1}{x-1}$.

Corollary 4. *For a chain with k n-gons G_k^n, the Tutte polynomial satisfies the following recurrent relation*

$$T(G_k^n;x,y) = \left(y + \frac{x^{n-1}-1}{x-1}\right) T(G_{k-1}^n;x,y) - y\,x^{n-2}\,T(G_{k-2}^n;x,y).$$

Corollaries 1 and 2 give two recurrent expressions of the Tutte polynomial.

Corollary 5. [11] *For the Tutte polynomial of a chain with k n-gons G_k^n,*

$$T(G_k^n;x,y) = c_n^{k-1}\left(y + x\,\frac{x^{n-1}-1}{x-1}\right) - d^{k-1}\,x\,,$$

where

$$\begin{pmatrix} c_n^k \\ d_n^k \end{pmatrix} = \begin{pmatrix} y + \dfrac{x^{n-1}-1}{x-1} & -1 \\ y\,x^{n-2} & 0 \end{pmatrix}^{k-1} \begin{pmatrix} y + \dfrac{x^{n-1}-1}{x-1} \\ y\,x^{n-2} \end{pmatrix}.$$

Applying Corollary 2, we have

Corollary 6. *For the Tutte polynomial of a chain with k n-gons G_k^n,*

$$T(G_k^n;x,y) = \frac{w_1}{2}\left(\frac{I+\sqrt{\Delta}}{2(x-1)}\right)^k - \frac{w_2}{2}\left(\frac{I-\sqrt{\Delta}}{2(x-1)}\right)^k,$$

where $I = x^{n-1} + y(x-1) - 1$,
$w_1 = \dfrac{xI - 2y(x-1)^2}{\sqrt{\Delta}} + x$ *and* $w_2 = \dfrac{xI - 2y(x-1)^2}{\sqrt{\Delta}} - x$,
$\Delta = x^{2n-2} - 2yx^n + 2(3y-1)x^{n-1} - 4yx^{n-2} + y^2x^2 - 2y(y+1)x + (y+1)^2$.

Let $T^*(z) = \sum_{k=0}^{\infty} T_k^n\, z^k$ be the generating function for T_k^n. From Corollary 3, we have

$$T^*(z) \;=\; \frac{x - y(x-1)\,z}{1 - \left(\dfrac{x^{n-1}-1}{x-1} + y\right) z \,+\, x^{n-2} y\, z^2},$$

that was obtained in Theorem 3.5 of [13].

4.2 Tutte polynomial for small chains

Now we apply the above formulae for trigonal, tetragonal, pentagonal, and hexagonal polycyclic chains.

4.2.1 Trigonal chains

By Corollary 6, the Tutte polynomial can be written for a chain G_k^3 with k triangles as

$$T(G_k^3;x,y) = \frac{w_1}{2}\left(\frac{I+\sqrt{\Delta}}{2}\right)^k - \frac{w_2}{2}\left(\frac{J-\sqrt{\Delta}}{2}\right)^k,$$

where $I = x+y+1$, $w_1 = \dfrac{xI - 2y(x-1)}{\sqrt{\Delta}} + x$ and $w_2 = \dfrac{xI - 2y(x-1)}{\sqrt{\Delta}} - x$,
$\Delta = x^2 - 2(y-1)x + 1 + 2y + y^2$.

The generation function for the Tutte polynomial $T_k^3 = T(G_k^3; x, y)$ can be presented in the form

$$T^*(z) \;=\; \frac{x - y(x-1)\,z}{1-(x+1+y)\,z \;+\; x\,y\,z^2}\,.$$

4.2.2 Tetragonal chains

For a chain G_k^4 with k quadrangles, we have

$$T(G_k^4; x, y) = \frac{w_1}{2}\left(\frac{I+\sqrt{\Delta}}{2}\right)^k - \frac{w_2}{2}\left(\frac{I-\sqrt{\Delta}}{2}\right)^k$$

where $I = x^2 + x + y + 1$, $w_1 = \dfrac{xI - 2y(x-1)}{\sqrt{\Delta}} + x$ and $w_2 = \dfrac{xI - 2y(x-1)}{\sqrt{\Delta}} - x$,
$\Delta = x^4 + 2x^3 - (2y-3)x^2 + 2(y+1)x + 1 + 2y + y^2$.

The generation function for the Tutte polynomial of tetragonal chains is

$$T^*(z) \;=\; \frac{x - y(x-1)\,z}{1-(x^2+x+1+y)\,z \;+\; x^2y\,z^2}\,.$$

4.2.3 Pentagonal chains

For a chain G_k^5 with k pentagons, we have

$$T(G_k^5; x, y) = \frac{w_1}{2}\left(\frac{I+\sqrt{\Delta}}{2}\right)^k - \frac{w_2}{2}\left(\frac{I-\sqrt{\Delta}}{2}\right)^k$$

where $I = x^3 + x^2 + x + y + 1$, $w_1 = \dfrac{xI - 2y(x-1)}{\sqrt{\Delta}} + x$ and $w_2 = \dfrac{xI - 2y(x-1)}{\sqrt{\Delta}} - x$,
$\Delta = x^6 + 2x^5 + 3x^4 - 2(y-2)x^3 + (2y+3)x^2 + 2(y+1)x + 1 + 2y + y^2$.

To obtain Tutte polynomial for pentagonal chains, one can use the generation function

$$T^*(z) \;=\; \frac{x - y(x-1)\,z}{1-(x^3+x^2+x+1+y)\,z \;+\; x^3y\,z^2}\,.$$

4.2.4 Hexagonal chains

This class of polycyclic chains include molecular graphs of unbranched benzenoid hydrocarbons [8]. For the Tutte polynomial of a chain G_k^6 with k hexagons,

$$T(G_k^6; x, y) = \frac{w_1}{2}\left(\frac{I+\sqrt{\Delta}}{2}\right)^k - \frac{w_2}{2}\left(\frac{I-\sqrt{\Delta}}{2}\right)^k \tag{9}$$

where $I = x^4+x^3+x^2+x+1+y$, $w_1 = \dfrac{xI - 2y(x-1)}{\sqrt{\Delta}} + x$ and $w_2 = \dfrac{xI - 2y(x-1)}{\sqrt{\Delta}} - x$,

$\Delta = x^8 + 2x^7 + 3x^6 + 4x^5 + (2y-5)x^4 + 2(y+2)x^3 + (2y+3)x^2 + 2(y+2)x + 1 + 2y + y^2.$

Formula (9) has been recently reported in [16].

The generation function for the Tutte polynomial for hexagonal chains of this class is

$$T^*(z) \;=\; \frac{x - y(x-1)\,z}{1 - (x^4 + x^3 + x^2 + x + 1 + y)\,z \;+\; x^4 y\, z^2}\,.$$

5 Negami polynomial

The Negami polynomial $N(G;t,x,y)$ for a graph G was introduced in [22]. It tells us many information about graph structure like the Tutte polynomial. The Negami polynomial was applied for constructing polynomials for spatial graphs, i.e., graphs knottedly embedding into three-dimensional space [12, 33, 36].

5.1 General expressions

Negami polynomial $N(G;t,x,y)$ for a graph G can be written as

$$N(G;t,x,y) \;=\; \sum_{Y\subset E(G)} t^{w(G-Y)}\, x^{q(G-Y)}\, y^{q(Y)}.$$

where $\omega(G)$ is the number of connected components of G and $p(G)$, $q(G)$ are the numbers of vertices and edges in G, respectively. This polynomial satisfies the following recurrent relation:

$$N(G;t,x,y) \;=\; x\,N(G/e;t,x,y) \;+\; y\,N(G-e;t,x,y),$$

where e is an arbitrary edge of a graph G.

For graphs $H\cdot K$, T_1 and L_1, we have $N(H\cdot K;t,x,y) = \dfrac{1}{t}\,N(H;t,x,y)\,N(K;t,x,y)$, $N(T_1;t,x,y) = t(x+ty)$ and $N(L_1;t,x,y) = t(x+y)$.

The polynomial $N(G;t,x,y)$ expands generally into

$$N(G;t,x,y) \;=\; \sum_{i=0}^{q}\sum_{j=1}^{p} m_{ij}\, t^j\, x^{q-i}\, y^i,$$

where m_{ij} is equal to the number of subsets Y of i edges in $E(G)$ such that $G-Y$ has precisely j connected components.

The Negami polynomial is a 2-invariant of graphs. Hence, the properties of function f and Negami polynomial are the same under the coefficients: $A = x$, $B = y$, $C = 1/t$, $D = t(x+ty)$, $E = t(x+y)$. For other quantities from Theorem 2, we have $a_n = \dfrac{1}{t}\left((x+ty)^{n-1} - x^{n-1}\right) + (x+y)x^{n-2}$, $b_n = x^{n-2}y\,(x+ty)^{n-2}(x+y)$, $f_0^n = t\,(x+ty)$, and $f_1^n = (x+ty)^n \;+\; (t-1)\,x^n$.

Corollary 7. [10] *For a chain with k n-gons G_k^n, the Negami polynomial satisfies the following recurrent relation*

$$\begin{aligned} N(G_k^n;t,x,y) &= \left((x+y)\,x^{n-2} + \frac{(x+ty)^{n-1}-x^{n-1}}{t}\right) N(G_{k-1}^n;t,x,y) \\ &\quad - y(x+y)x^{n-2}\,(x+ty)^{n-2}\,N(G_{k-2}^n;t,x,y). \end{aligned}$$

Corollary 8. [10] *For a chain with k n-gons G_k^n, the Negami polynomial satisfies the following recurrent relation*

$$N(G_k^n;t,x,y) = c_n^{k-1}\,f_1^n \;-\; d_n^{k-1}\,f_0^n,$$

where

$$\begin{pmatrix} c_n^k \\ d_n^k \end{pmatrix} = \begin{pmatrix} a_n & -1 \\ b_n & 0 \end{pmatrix}^{k-1} \begin{pmatrix} a_n \\ b_n \end{pmatrix}.$$

Corollary 9. *For the Negami polynomial of a chain with k n-gons G_k^n,*

$$N(G_k^n;t,x,y) = \frac{w_1}{2}\left(\frac{I+\sqrt{\Delta}}{2t(x+ty)}\right)^k - \frac{w_2}{2}\left(\frac{I-\sqrt{\Delta}}{2t(x+ty)}\right)^k,$$

where $I = (t-1)x^n + t^2x^{n-2}y(x+y) + (x+ty)^n$,

$$w_1 = \frac{t(x+ty)(I-2t^2x^{n-2}y(x+y))}{\sqrt{\Delta}} + t(x+ty),$$

$$w_2 = \frac{t(x+ty)(I-2t^2x^{n-2}y(x+y))}{\sqrt{\Delta}} - t(x+ty),$$

$$\begin{aligned} \Delta &= (x+ty)^{2n} + 2x^{n-2}(tx+ty-x)(x+ty)^{n+1} - 4\,t^2x^{n-2}y(x+y)(x+ty)^n \\ &\quad + x^{2n-4}\big[2\,t^2(t-1)x^2y(x+y) + t^4y^2(x+y)^2 + (t-1)^2x^4\big]. \end{aligned}$$

Let $N^*(z) = \sum_{k=0}^{\infty} N_k^n\,z^k$ be the generating function for the Negami polynomial. Then

$$N^*(z) = \frac{t(x+ty) - t^2x^{n-2}y(x+y)z}{1 - \dfrac{(x+ty)^{n-1} + x^{n-2}(tx+ty-x)}{t}\,z + \left[x^{n-2}y(x+y)(x+ty)^{n-2}\right]z^2}.$$

5.2 Negami polynomial for small chains

Now we apply the above formulas for polycyclic chains of U_k^n, $n \le 6$.

5.2.1 Trigonal chains

By Corollary 9, the Negami polynomial can be written for trigonal chains with k triangles as

$$N(G_k^3;x,y)=\frac{w_1}{2}\left(\frac{I+\sqrt{\Delta}}{2}\right)^k-\frac{w_2}{2}\left(\frac{I-\sqrt{\Delta}}{2}\right)^k,$$

where $I=x^2+3xy+ty^2$, $\Delta=x^4+2x^3y-(2t-5)x^2y^2+2txy^3+t^2y^4$,

$$w_1=\frac{t(x+ty)I-2t^2xy(x+y)}{\sqrt{\Delta}}+t(x+ty),$$

$$w_2=\frac{t(x+ty)I-2t^2xy(x+y)}{\sqrt{\Delta}}-t(x+ty).$$

To obtain Negami polynomials, one can apply the generation function

$$N^*(z)=\frac{(x+ty)-t^2xy(x+y)z}{1-(x^2+3xy+ty^2)z+xy(x+y)(x+ty)z^2}.$$

5.2.2 Tetragonal chains

For graphs G_k^4, we have

$$N(G_k^4;x,y)=\frac{w_1}{2}\left(\frac{I+\sqrt{\Delta}}{2}\right)^k-\frac{w_2}{2}\left(\frac{I-\sqrt{\Delta}}{2}\right)^k$$

where $I=x^3+4yx^2+3ty^2x+t^2y^3$,

$\Delta=x^6+4x^5y-2(t-6)x^4y^2-2t(t-8)x^3y^3+13t^2x^2y^4+6t^3xy^5+t^4y^6$,

$$w_1=\frac{t(x+ty)I-2t^2x^2y(x+y)}{\sqrt{\Delta}}+t(x+ty),$$

$$w_2=\frac{t(x+ty)I-2t^2x^2y(x+y)}{\sqrt{\Delta}}-t(x+ty)$$

To obtain Negami polynomials, one can apply the generation function.

$$N^*(z)=\frac{(x+ty)-t^2x^2y(x+y)z}{1-(x^3+4x^2y+3txy^2+t^2y^3)z+x^2y(x+y)(x+ty)^2z^2}.$$

5.2.3 Pentagonal chains

For chains G_k^5 with k 5-gons, we have

$$N(G_k^5;x,y)=\frac{w_1}{2}\left(\frac{I+\sqrt{\Delta}}{2}\right)^k-\frac{w_2}{2}\left(\frac{I-\sqrt{\Delta}}{2}\right)^k$$

where $I=x^4+5x^3y+6tx^2y^2+4t^2xy^3+t^3y^4$,

$\Delta=x^8+6x^7y+21x^6y^2-4t(t-12)x^5y^3-2t^2(t-32)x^4y^4+54t^3x^3y^5+28t^4x^2y^6+8t^5xy^7+t^6y^8$,

$$w_1 = \frac{t(x+ty)I - 2t^2x^3y(x+y)}{\sqrt{\Delta}} + t(x+ty),$$
$$w_2 = \frac{t(x+ty)I - 2t^2x^3y(x+y)}{\sqrt{\Delta}} - t(x+ty).$$

To obtain Negami polynomials, one can apply the generation function.

$$N^*(z) = \frac{(x+ty) - t^2x^3y(x+y)z}{1-(x^4+5x^3y+6tx^2y^2+4t^2xy^3+t^3y^4)z + x^3y(x+y)(x+ty)^3z^2}.$$

5.2.4 Hexagonal chains

For chains G_k^6 with k 6-gons, we have

$$N(G_k^6;x,y) = \frac{w_1}{2}\left(\frac{I+\sqrt{\Delta}}{2}\right)^k - \frac{w_2}{2}\left(\frac{I-\sqrt{\Delta}}{2}\right)^k$$

where $I = x^5 + 6x^4y + 10tx^3y^2 + 10t^2x^2y^3 + 5t^3xy^4 + t^4y^5$,

$$\Delta = x^{10} + 8x^9y + 4(t+8)x^8y^2 - 4t(t-28)x^7y^3 - 2t^2(3t-98)x^6y^4 - 2t^3(t-122)x^5y^5$$
$$+ 208t^4x^4y^6 + 120t^5x^3y^7 + 45t^6x^2y^8 + 10t^7xy^9 + t^8y^{10},$$
$$w_1 = \frac{t(x+ty)I - 2t^2x^4y(x+y)}{\sqrt{\Delta}} + t(x+ty),$$
$$w_2 = \frac{t(x+ty)I - 2t^2x^4y(x+y)}{\sqrt{\Delta}} - t(x+ty).$$

To obtain Negami polynomials, one can apply the generation function.

$$N^*(z) = \frac{(x+ty) - t^2x^4y(x+y)z}{1-(x^5+6x^4y+10tx^2y^2(x+ty)+5t^3xy^4+t^4y^5)z + x^4y(x+y)(x+ty)^4z^2}.$$

In conclusion, we give relations between the Tutte and the Negami polynomials [22, 24]. If graph G has p vertices, q edges and ω connected components, then

$$T(G;x,y) = (x-1)^{-\omega}\,(y-1)^{-p}\;N(G;(x-1)(y-1),1,y-1),$$
$$N(G;t,x,y) = (tyx^{-1})^{\omega}\,(xy^{-1})^p\,y^q\;T(G;1+tyx^{-1},1+xy^{-1}).$$

6 Yamada polynomial

Yamada polynomial $h(G;x,y)$ of a graph G have been introduced in [36] for constructing a polynomial of graphs knottedly embedded in the three-dimensional space. It is a Laurent polynomial and can be presented as

$$h(G;x,y) \;=\; \sum_{Y\subset E(G)} (-x)^{-|Y|}x^{\omega(G-Y)}y^{\beta(G-Y)},$$

where the summation goes over all edge subsets Y of $E(G)$, $\omega(G)$ is the number of connected components in G, and $\beta(G)$ is the cyclomatic number of a graph, $\beta(G) = q(G) - p(G) + \omega(G)$.

This polynomial $h(G;x,y)$ satisfies the recursive expression

$$h(G;x,y) \;=\; h(G/e;x,y) \;-\; \frac{1}{x}\,h(G-e;x,y).$$

and has the following properties: $h(G \cdot H;x,y) = \frac{1}{x}h(G;x,y) \cdot h(H;x,y)$, $h(T_1;x,y) = 0$, and $h(L_1;x,y) = xy - 1$. Therefore, properties of f and $h(G;x,y)$ coincide under the coefficients: $A = 1$, $B = -1/x$, $C = 1/x$, $D = 0$, and $E = xy - 1$. For other quantities from Theorem 2, we have $a_n = y - 2/x$, $b_n = 0$, $c_n^{k-1} = a_n^{k-1}$, $d_n^{k-1} = 0$, $f_0^n = 0$ and $f_1^n = xy - 1$.

Corollary 10. *For a chain with k n-gons G_k^n, the Yamada polynomial satisfies the following recurrent relation*

$$h(G_k^n;x,y) = \left(y - \frac{2}{x}\right) h(G_{k-1}^n;x,y).$$

The Yamada polynomial characterizes polycyclic chains irrespective of the size of its rings. It follows from the fact that $h(G_k^n;x,y)$ does not distinguish between homeomorphic graphs.

Corollary 11. *Let a chain G_k consists of k polygons, i.e., $G_k \in \cup_{n\ge 3} U_k^n$. Then*

$$h(G_k;x,y) = \left(y - \frac{2}{x}\right)^{k-1} (xy - 1).$$

Denote $h_k = h(G_k;x,y)$ and let $h^*(z) = \sum_{k=0}^{\infty} h_k\, z^k$ be the generating function. Then

$$h^*(z) \;=\; \frac{(xy-1)\,z}{1 - \left(y - \dfrac{2}{x}\right)\,z}\,.$$

One can see that the Yamada polynomial is the same for all $n \ge 3$, i.e., for all homeomorphic chains.

For a graph G with p vertices, the Yamada polynomial can be expressed through the Negami polynomial. Namely, $h(G;x,y) = y^{-p}\,N(G;xy,y,-x^{-1})$.

7 The chromatic polynomial

The chromatic polynomial $P(G;x)$ is a one-variable polynomial such that, for all integer positive values of x, $P(G;x)$ is equal to the number of proper colorings of G with x colors [25, 26, 31, 32]. A recursive formula for $P(G;x)$ is as follow:

$$P(G;x) \;=\; -\,P(G/e;x) \;+\; P(G-e;x),$$

where e is not a loop. For graphs $H \cdot K$, T_1, L_1, we have $P(H \cdot K;x) = \frac{1}{x}\,P(H;x)\,P(K;x)$, $P(T_1;x) = x(x-1)$ and $P(L_1;x) = 0$. Therefore, the properties of f and $P(G;x)$ coincide under the coefficients: $A = -1$, $B = 1$, $C = 1/x$, $D = x(x-1)$, and $E = 0$. Besides, we can write $a_n = \dfrac{1}{x}\left((x-1)^{n-1} - (-1)^{n-1}\right)$, $b_n = 0$, $c_n^{k-1} = a_n^{k-1}$, $d_n^{k-1} = 0$, $f_0^n = x\,(x-1)$ and $f_1^n = x\,(x-1)\,a_n$.

As a result we obtain the simple formulae which also follow from other properties of the polynomial [32].

Corollary 12. *For a chain with k n-gons G_k^n, the chromatic polynomial satisfies the following recurrent relation*

$$P(G_k^n;x) = \frac{1}{x}\left[(x-1)^{n-1} \;-\; (-1)^{n-1}\right]P(G_{k-1}^n;x)$$

Corollary 13. *The chromatic polynomial may be presented in the form*

$$P(G_k^n;x) = x\,(x-1)\left(\frac{(x-1)^{n-1} - (-1)^{n-1}}{x}\right)^k.$$

Denote $P_k^n = P(G_k^n;x)$ and let $P^*(z) = \sum\limits_{k=0}^{\infty} P_k^n\,z^k$ be the generating function. Then

$$P^*(z) \;=\; \frac{x^2(x-1)}{x + \left[(-1)^{n-1} - (x-1)^{n-1}\right]z}.$$

The chromatic polynomial can be regarded as specialization of the Tutte and the Negami polynomials. For a graph G with p vertices, q edges and ω connected components,

$P(G;x) = (-1)^{p-\omega}\,x^{\omega}\,T(G;1-x,0)$,

$P(G;x) = N(G;x,-1,1)$.

8 The flow polynomial

For the flow polynomial $F(G;x)$, the recursive formula is written as [19, 32]:

$$F(G;x) = F(G/e;x) - F(G-e;x).$$

where e is not a loop. Further, for graphs $H \cdot K$, T_1 and L_1, the equations $F(H \cdot K;x) = F(H;x)\,F(K;x)$, $F(T_1;x) = 0$, and $F(L_1;x) = x-1$ hold. Then the properties of f and $F(G;x)$ are the same under the coefficients: $A = 1$, $B = -1$, $C = 1$, $D = 0$, $E = x-1$. For other quantities from Theorem 2, $a_n = x-2$, $b_n = 0$, $c_n^{k-1} = a_n^{k-1}$, $d_n^{k-1} = 0$, $f_0^n = 0$ and $f_1^n = x-1$. Hence, the flow polynomial satisfies the following recurrent relation for chains with k n-gons:

$$F(G_k^n;x) = (x-2)\,F(G_{k-1}^n;x).$$

This immediately implies

$$F(G_k^n;x) = (x-1)\,(x-2)^{k-1}.$$

One can see that the flow polynomial is the same for all $n \geq 3$, i.e., for all homeomorphic chains. Ii follows also from the fact that $F(G_k^n;x)$ is the specific case of the Yamada polynomial at $x = 1$ and $y = x$.

Denote $F_k = F(G_k;x)$, $G_k \in \cup_{n\geq 3} U_k^n$, and let $F^*(z) = \sum_{k=0}^{\infty} F_k\, z^k$ be the generating function. Then

$$F^*(z) = \frac{(x-1)\,z}{1-(x-2)\,z}.$$

The flow polynomial can be calculated through the Tutte and the Negami polynomials for a graph G with p vertices, q edges and ω connected components:

$F(G;x) = (-1)^{q-p+\omega}\,T(G;0,1-x)$,

$F(G;x) = x^{-p}\,N(G;x,x,-1)$.

9 Conclusion

We have considered a general calculation scheme for the polynomial graph invariant f based on edge deletion and contraction in a graph. For chains of polygons, recurrent and explicit formulae of the invariant have been presented.

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