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ORIGINAL PAPER

Planar polycyclic graphs and their Tutte polynomials

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Abstract We consider several classes of planar polycyclic graphs and derive recurrences satisfied by their Tutte polynomials. The recurrences are then solved by computing the corresponding generating functions. As a consequence, we obtain values of several chemically and combinatorially interesting enumerative invariants of considered graphs. Some of them can be expressed in terms of values of Chebyshev polynomials of the second kind.

1 Introduction

A deletion-contraction invariant of a graph G is an invariant that satisfies and can be computed *via* some kind of deletion-contraction recurrence over the edges of G. The Tutte polynomial is the most general such invariant. It is a powerful analytic tool that encodes important information about the graph. The chromatic polynomial, the flow polynomial, and the tension polynomial all arise as its specializations, and its special evaluations yield several important enumerative invariants, such as, e.g., the number of spanning trees, the number of connected subgraphs, the number of acyclic orientations, etc. In this paper we compute the generating function for the Tutte polynomials of a class of polygonal chains and show that many enumerative invariants of such graphs can be expressed as values of Chebyshev polynomials of the second kind.

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2 Definitions and preliminaries

2.1 Tutte polynomial

We say that $\tau(G)$ is a **deletion-contraction invariant** of G if it can be computed by performing a series of deletions and contractions of edges of G. The deletion of an edge $e \in E(G)$ results in the graph $G - e$ on the same set of vertices without e, while the contraction of e results in the graph G/e in which e is removed and its end-vertices are identified. Typical examples of such invariants are the number of spanning trees $\tau(G)$ and the chromatic polynomial $\chi(G, \lambda)$. The respective recurrences are

$$\tau(G) = \tau(G - e) + \tau(G/e)$$

and

$$\chi(G, \lambda) = \chi(G - e, \lambda) - \chi(G/e, \lambda).$$

The initial conditions are usually specified for empty graphs (i.e., the graphs without edges) and/or for graphs with only loops and/or bridges.

The Tutte polynomial $T(G; x, y)$ of a graph G is, in a sense, the most general invariant of this type. It can be defined in terms of Whitney's rank generating function of G [10], but we find more convenient an equivalent definition that emphasizes its deletion-contraction nature. It was introduced in 1954 by Tutte [8], who also established some of its basic properties [9]. For a more thorough introduction we refer the reader to the final chapter of [1].

The **Tutte polynomial** of a graph G is defined as

$$T(G; x, y) = \begin{cases} 1 & \text{if } E(G) \text{ is empty} \\ x \cdot T(G/e; x, y) & \text{if e is a bridge} \\ y \cdot T(G - e; x, y) & \text{if e is a loop} \\ T(G - e; x, y) + T(G/e; x, y) & \text{if e is any other edge.} \end{cases}$$

It is clear that $T(G; x, y)$ has nonnegative integer coefficients and it can be shown that the definition is independent of the choice of e.

It is clear from the definition that the Tutte polynomial of any forest G with m edges is given by $T(G; x, y) = x^m$. Similarly, if G is a graph with one vertex and r loops, then $T(G; x, y) = y^r$. It follows easily by induction on n that the Tutte polynomial of the cycle on n vertices is

$$T(C_n; x, y) = x^{n-1} + \cdots + x^2 + x + y.$$

By exchanging the roles of x and y we obtain the Tutte polynomial of the graph on two vertices connected by n parallel edges, the dual graph of C_n. It turns out that this is valid for all planar graphs.

Theorem 2.1 *Let G be a planar graph and G^* its dual. Then $T(G; x, y) = T(G^*; y, x)$.*

We quote another property that will be useful in the rest of the paper.

Theorem 2.2 *The Tutte polynomial of a graph G is equal to the product of Tutte polynomials of its blocks. (A block is a maximal connected subgraph of G without a cut-vertex.)*

We conclude this subsection by listing some special evaluations of Tutte polynomials that yield enumerative invariants of G. We refer the reader to [1] for definitions of the terms not given here. In order to avoid terminological ambiguities, we suppose that G is a connected graph. Then:

$T(G; 1, 1)$ is the number of spanning trees of G;
$T(G; 2, 1)$ is the number of spanning forests of G;
$T(G; 1, 2)$ is the number of connected spanning subgraphs of G;
$T(G; 0, 2)$ is the number of strongly connected orientations of G;
$T(G; 2, 0)$ is the number of acyclic orientations of G;
$T(G; 1, 0)$ is the number of acyclic orientations of G with a single source;
$T(G; 2, 2) = 2^{|E(G)|}$.

It is clear from the above list that it is highly desirable to know the Tutte polynomial, since it encodes a wealth of combinatorial information about the graph. However, it is not easy, since in the general case the complexity can be exponentially high. Fortunately, for several classes of chemically interesting graphs there exist efficient methods that yield explicit formulas for their Tutte polynomials.

2.2 Polygonal chains and other planar polycyclic graphs

In this subsection and in the rest of the paper we consider planar graphs whose all bounded faces are cycles. The class is broad enough to include several chemically interesting families, such as cacti, polyphenylenes, and benzenoid chains.

A **cactus graph** is a connected graph in which no edge is contained in more than one cycle. Hence, each block of a cactus graph is either a cycle or an edge. A cactus graph in which all blocks are cycles of the same size m is called m-uniform cactus graph. For example, 6-uniform cactus is called a **hexagonal cactus**. A **polyphenylene** is a graph obtained from a hexagonal cactus by expanding each of its cut-vertices to an edge. A polyphenylene (a cactus) in which no hexagon has more than two cut-vertices is called a **polyphenylene chain** (a cactus chain). For more information on enumerative invariants of chemically interesting cacti and polyphenylenes we refer the reader to references [3,4].

The **interior dual** G^0 of a planar graph G is obtained from the dual graph G^* by omitting the vertex corresponding to the unbounded face and all incident edges. It is clear from the definition that inner duals of cacti and polyphenylene are disconnected graphs. If the interior dual of a planar graph G is a tree, we say that G is a **catacondensed polygonal cluster**; if G^0 is isomorphic to a path, we say that G is a **polygonal chain**. If all its faces are of the same size, we call the cluster or the chain **uniform**.

The number of bounded faces is called the length of the chain. The terminology is borrowed from benzenoid chemistry; the 6-uniform polygonal clusters are known as catacondensed benzenoid graphs, and similar for chains. We refer the reader to [6] for more information on benzenoid graphs.

The last class of graphs we consider here are book graphs. A **book graph** on n sheets is a collection of n cycles that all share exactly one of their edges. Again, if all cycles are of the same length, say k, we have a k-uniform book. The most interesting special case is $k = 4$, the Cartesian product of a star and K_2.

3 Main results

3.1 Cacti and polyphenylenes

Let G be a cactus graph with m bridges and n blocks B_i, where each B_i is a cycle of length k_i. The following result is a direct consequence of Theorem 2.2.

Theorem 3.1

$$T(G; x, y) = x^m \prod_{i=1}^{n} T(C_{k_i}; x, y).$$

If the cactus G is k-uniform, the above expression can be simplified.

Corollary 3.2 *Let $G_n(k)$ be a k-uniform cactus with n blocks. Then*

$$T(G_n(k); x, y) = (x^{k-1} + \cdots + x^2 + x + y)^n.$$

From Corollary 3.2 we can immediately read out a number of invariants.

Corollary 3.3 *Let $G_n(k)$ be a k-uniform cactus with n blocks. Then $G_n(k)$ has k^n spanning trees, $(k+1)^n$ connected spanning subgraphs, $(2^k - 1)^n$ spanning forests and $(2^k - 2)^n$ acyclic orientations.*

We see that all those invariants are insensitive to the positions of cut-vertices, while some other invariants, like the number of matchings and the number of independent sets, depend strongly on the distribution of cut-vertices [3,4]. This is not a great surprise, given the very weak nature of connectivity within cacti. In the next subsection we will see that this behavior is preserved also in polygonal chains.

3.2 Uniform polygonal chains

This subsection is the central part of the paper. In it we consider uniform polygonal chains and we study how their Tutte polynomials depend on their length. We show that the Tutte polynomials satisfy a two-term recurrence with polynomial coefficients. Such recurrences can be solved to derive the explicit formulas; however, we prefer to compute the corresponding generating functions. Our results complement and generalize those obtained in recent reference [5].

First we show that the Tutte polynomial does not depend on the shape of a chain.

Theorem 3.4 *Let $G_n(k)$ and $H_n(k)$ be two k-uniform polygonal chains of the same length n. Then $T(G_n(k); x, y) = T(H_n(k); x, y)$.*

Proof The claim follows from Theorem 2.1 and the fact that $G_n(k)$ and $H_n(k)$ have isomorphic duals. □

Now we can look at any k-uniform chain consisting of n cycles. By applying the deletion-contraction procedure on one of its terminal polygons, one can arrive at a two-term recurrence relation with polynomial coefficients. The procedure is completely analogous to the one described in reference [5] for benzenoid chains. In order to simplify the notation, we will omit k whenever it cannot lead to a confusion.

Theorem 3.5 *Let G_n be a k-uniform polygonal chain of length n. Then*

$$T(G_n; x, y) = p(x, y)T(G_{n-1}; x, y) + q(x, y)T(G_{n-2}; x, y),$$

where the coefficient polynomials are given as

$$p(x, y) = \frac{x^{k-1} - 1}{x - 1} + y, \qquad q(x, y) = -x^{k-2}y.$$

The initial conditions are

$$T(G_0; x, y) = T_0(x, y) = x, \qquad T(G_1; x, y) = T_1(x, y) = x\frac{x^{k-1} - 1}{x - 1} + y.$$

Proof Let e be any of $k - 1$ edges shared by one of the terminal polygons and the unbounded face. (We call such edges terminal.) Its deletion leaves G_{n-1} with $k - 2$ edges attached; since each of them is a cut-edge, the Tutte polynomial of $G_n - e$ is given by $x^{k-2} \cdot T(G_{n-1}; x, y)$. Contraction of e results in a graph G'_n consisting of G_{n-1} with a cycle of length $k-1$ attached along one of its terminal edges. By applying the deletion-contraction operation on one of the edges of terminal C_{k-1}, we obtain again a copy of G_{n-1}, this time with $k - 3$ cut-edges attached, and a new graph, G''_n, consisting of G_{n-1} with a cycle of length $k - 2$ attached at one end. We proceed until we arrive at a graph $G_n^{(k-2)}$ which is G_{n-1} with one of its terminal edge replaced by two parallel edges. By now we have

$$T(G_n; x, y) = (x^{k-2} + x^{k-3} + \cdots + x)T(G_{n-1}; x, y) + T(G_n^{(k-2)}; x, y).$$

Now, deleting one of the parallel terminal edges of $G_n^{(k-2)}$ leads to another copy of G_{n-1}, while its contraction results in G'_{n-1} with one loop attached to one if its terminal vertices. Hence,

$$T(G_n; x, y) = (x^{k-2} + x^{k-3} + \cdots + x + 1)T(G_{n-1}; x, y) + y \cdot T(G'_{n-1}; x, y).$$

The claim now follows by noticing that

$$T(G'_{n-1}; x, y) = T(G_{n-1}; x, y) - x^{k-2} \cdot T(G_{n-2}; x, y),$$

collecting the terms and expressing the results in a compact form. □

From the above recurrence one could, in principle, obtain explicit formulas for $T(G_n; x, y)$. However, the obtained expression tend to be rather complicated. An example (for $k = 6$) can be found in [5]. Instead, we prefer to compute the generating function for the Tutte polynomials of G_n.

The **generating function** $F(t)$ of a sequence f_n is a formal power series $F(t) = \sum_{n=0}^{\infty} f_n t^n$. Generating functions of sequences of polynomials are defined analogously. For example, the generating function of the sequence of Chebyshev polynomials of the second kind $U_n(x)$ is given by

$$U(x, t) = \sum_{n=0}^{\infty} U_n(x) t^n = \frac{1}{1 - 2xt + t^2}.$$

Let us denote by $T(x, y, t)$ the generating function of the sequence $T(G_n; x, y)$, i.e.,

$$T(x, y, t) = \sum_{n=0}^{\infty} T(G_n; x, y) t^n.$$

By a straightforward computation we obtain the following result.

Theorem 3.6

$$T(x, y, t) = \frac{x - (x-1)yt}{1 - p(x, y)t - q(x, y)t^2}.$$

Now, by substituting special values of x and y, we obtain the generating functions for the enumerative invariants mentioned in the introduction. In many cases the resulting expressions can be interpreted in terms of values of Chebyshev polynomials.

Corollary 3.7 *Let G_n be a k-uniform polygonal chain of length n. Then*

(a) The number of acyclic orientations of G_n with a single source is $(k-1)^n$;
(b) The total number of acyclic orientations of G_n is given by $2(2^{k-1} - 1)^n$;
(c) The number of strongly connected cyclic orientations of G_n is $2 \cdot 3^{n-1}$;
(d) The number of spanning trees in G_n is $U_n(k/2)$;
(e) The number of connected spanning subgraphs of G_n is $2^{n/2} U_n\left(\frac{k+1}{2\sqrt{2}}\right)$;
(f) The number of spanning forests of G_n is $\left(\sqrt{2}^{k-2}\right)^{n-1} U_{n+1}\left(\sqrt{2}^{k-2}\right)$.

The proof follows by substituting the corresponding values of x and y and interpreting the obtained generating functions in terms of powers and/or Chebyshev polynomials. The above values are listed approximately in order of increasing complexity.

For the case of benzenoid chains we list explicitly the numbers of various classes of spanning subgraphs.

Corollary 3.8 *Let G_n be a benzenoid chain of length n. Then*

(a) The number of spanning trees in G_n is $U_n(3)$;

(b) The number of connected spanning subgraphs of G_n is $2^{n/2}U_n\left(\frac{7}{2\sqrt{2}}\right)$;

(c) The number of spanning forests of G_n is $4^{n-1}U_{n+1}(4)$.

All results follow from specializing x and y in the generating function for the Tutte polynomials of benzenoid chains,

$$T_B(x, y, t) = \frac{x + (x-1)yt}{1 - (x^4 + x^3 + x^2 + x + 1 + y)t + x^4yt^2}.$$

The chemical and combinatorial interpretation of sequences enumerating the connected spanning subgraphs and spanning forests seem to be new; the first one appears as sequence A186446 in the *Online Encyclopedia of Integer Sequences* [7] without any comments, while the second one is not there. The sequence enumerating the spanning trees has many combinatorial interpretations (sequence A001109 of [7]), some of them even chemically relevant ([2], pp. 301, 302), but the number of spanning trees of a benzenoid chain is not mentioned.

For some other values of k we obtain familiar sequences, but their interpretation in terms of spanning subgraphs of polygonal chains also seems to be new. For example, no interpretation in terms of the number of spanning trees and forests is mentioned for sequences A001906 (the even-indexed Fibonacci numbers) and A003480 that count them in $G_n(3)$. The exception seems to be the case $k = 4$, where both sequences counting spanning trees and spanning forests are recognized in [7] as sequences A001353 and A022026, respectively.

3.3 Book graphs

The main difference between the (uniform) polygonal chains and the (uniform) book graphs is that in the former case there are two special, terminal, cycles, while in the case of books all their sheets are equivalent. Nevertheless, their Tutte polynomials satisfy similar recurrences. For the case of simplicity, we consider here only 4-uniform books, but the results could be easily verified for other values of k.

Theorem 3.9 *Let B_n be a* 4*-uniform book on n sheets. Then the Tutte polynomials of B_n satisfy the two-term linear recurrence with polynomial coefficients*

$$\begin{aligned} T(B_n; x, y) = &(2x^2 + 2x + 1 + y)T(B_{n-1}; x, y) \\ &-(x^2 + x + 1)(x^2 + x + y)T(B_{n-2}; x, y) \end{aligned}$$

with the initial conditions

$$T(B_1; x, y) = x^3 + x^2 + x + y, \qquad T(B_0; x, y) = x.$$

Proof We start by selecting any of n cycles C_4 and applying the deletion-contraction procedure to any of its edges that is not shared with other cycles. This results in B_{n-1}

with two cut-edges attached and in B'_n, consisting of B_n with one C_4 replaced by a triangle. By deleting and contracting an edge of that triangle we obtain B_{n-1} with one cut-edge attached and B''_n, that is B_{n-1} with the central edge (the "spine of the book") replaced by two parallel edges. Finally, by deleting and contracting one of those parallel edges we obtain another copy of B_{n-1} and a set of $n-1$ triangles sharing a vertex with a loop attached at that vertex. In terms of Tutte polynomials, it reads as

$$T(B_n; x, y) = (x^2 + x + 1)T(B_{n-1}; x, y) + y \cdot T(C_3; x, y)^{n-1}.$$

This is a non-homogeneous linear recurrence of the first order. It can be made homogeneous by writing it for $T(B_{n-1}; x, y)$, multiplying it through by $T(C_3; x, y)$ and then subtracting it from the original recurrence. The result is the recurrence stated in the theorem. □

It is a matter of routine computation to obtain the generating function for $T(B_n; x, y)$.

Theorem 3.10

$$\begin{aligned} B(x, y, t) &= \sum_{n=0}^{\infty} T(B_n; x, y)t^n \\ &= \frac{x - (x^3 + x^2 + xy + y)t}{1 - (2x^2 + 2x + 1 + y)t + (x^2 + x + 1)(x^2 + x + y)t^2} \end{aligned}$$

The number of spanning trees of B_n can now be obtained by taking $x = y = 1$. That yields the generating function $\frac{1-2t}{(1-3t)^2}$ whose coefficients count the spanning trees.

Corollary 3.11

$$\tau(B_n) = (n + 3)3^{n-1}$$

The sequence $(n+3)3^{n-1}$ appears as A006234 in [7], and the number of spanning trees of B_n is mentioned as a conjectured combinatorial interpretation. Hence our result proves that conjecture. We mention in passing that $\tau(B_n)$ can be also expressed in terms of Chebyshev polynomials, $\tau(B_n) = 3^{n-1}U_{n+2}(1)$.

We leave the derivation of recurrence for other values of k to the interested reader.

4 Concluding remarks

The Tutte polynomial encodes a wealth of combinatorial information about the underlying graph. In this paper we have computed Tutte polynomials for many chemically interesting graphs, such as cacti, polyphenylenes and benzenoid chains. We have shown that several classes of spanning subgraphs of such graphs are enumerated by sequences of values of Chebyshev polynomials, thus providing new combinatorial interpretations for those sequences. In particular, we have proved a conjecture about the number of spanning trees in the Cartesian product of a star and K_2.

The methods applied here could also be used to compute Tutte polynomials (and hence enumerative invariants) for some other chemically interesting graphs such as, e.g., phenylene chains and prisms. They could, in principle, also be applied to branched polymers, but it seems that the recurrences get more and more complicated. Nevertheless, it might be worth trying at least for some special cases.

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References

1. B. Bollobás, *Modern Graph Theory*, Graduate Texts in Mathematics 184. (Springer, Berlin, 1998)
2. S.J. Cyvin, I. Gutman *Kekulé structures in benzenoid hydrocarbons*, Lecture Notes in Chemistry 46, (Springer, New York, 1988)
3. T. Došlić, F. Maløy, Chain hexagonal cacti: matchings and independent sets. Discrete Math. **310**, 1176–1190 (2010)
4. T. Došlić, M.-S. Litz, Matchings and independent sets in polyphenylene chains. MATCH Commun. Math. Comput. Chem. **67**, 313–330 (2012)
5. G.H. Fath-Tabar, Z. Gholam-Rezaei, A.R. Ashrafi, On the Tutte polynomial of benzenoid chains. Iran. J. Math. Chem. **3**, 113–119 (2012)
6. I. Gutman, S.J. Cyvin, *Introduction to the Theory of Benzenoid Hydrocarbons* (Springer, Berlin, 1989)
7. The Online Encyclopedia of Integer Sequences, http://oeis.org
8. W.T. Tutte, A contribution to the theory of chromatic polynomials. Can. J. Math. **6**, 80–91 (1954)
9. W.T. Tutte, On dichromatic polynomials. J. Comb. Theory **2**, 301–320 (1967)
10. H. Whitney, The coloring of graphs. Ann. Math. **33**, 688–718 (1932)