



Also available at http://amc-journal.eu ISSN 1855-3966 (printed edn.), ISSN 1855-3974 (electronic edn.) ARS MATHEMATICA CONTEMPORANEA 11 (2016) 255–276

Counting maximal matchings in linear polymers

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Received 15 May 2015, accepted 24 October 2015, published online 30 November 2015

Abstract

A matching M in a graph G is maximal if it cannot be extended to a larger matching in G. In this paper we show how several chemical and technical problems can be successfully modeled in terms of maximal matchings. We introduce the maximal matching polynomial and study its basic properties. Then we enumerate maximal matchings in several classes of graphs made by a linear or cyclic concatenation of basic building blocs. We also count maximal matchings in joins and corona products of some classes of graphs.

Keywords: Maximal matching, maximal matching polynomial, cactus graph, cactus chain, Padovan numbers, Perrin numbers, corona product.

Math. Subj. Class.: 05C30, 05C70

1 Introduction

Many problems in natural, technical and social sciences can be successfully formulated in terms of matchings in graphs. Today the matching theory is a well developed branch of graph theory, studying both structural and enumerative aspects of matchings. Its development has been strongly stimulated by chemical applications, in particular by the study of perfect matchings in benzenoid graphs. Additional impetus came with discovery of fullerenes, again mostly dealing with perfect matchings [5, 6, 22, 30], but including also some structural results [1,7].

For a general background on matching theory and terminology we refer the reader to the classical monograph by Lovász and Plummer [24]. For graph theory terms not defined here we also recommend [29].

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A matching M in a graph G is a collection of edges of G such that no two edges from M share a vertex. The cardinality of M is called the **size** of the matching. As the matchings of small size are not interesting (each edge is a matching of size one, and the empty set is the unique matching of size 0), we will be mostly interested in matchings that are, in a sense, "large". Most often, we are interested in matchings that are as large as possible.

A matching M is **maximum** if there is no matching in G with more edges than M. The cardinality of any maximum matching in G is called the **matching number** of G and denoted by $\nu(G)$. Since each vertex can be incident to at most one edge of a matching, it follows that the matching number of a graph on n vertices cannot exceed $\lfloor n/2 \rfloor$. If each vertex of G is incident with an edge of M, the matching M is called **perfect**. Perfect matchings are obviously also maximum matchings. The perfect matchings, also known as **Kekulé structures** in chemical literature, have played a central role in the study of matchings for several decades.

There is, however, an alternative way to quantify the idea of "large" matchings. A matching M in G is **maximal** if no other matching in G contains it as a proper subset. Obviously, every maximum matching is also maximal, but the opposite is generally not true.

Maximal matchings are much less researched that their maximum counterparts. That goes both for their structural and their enumerative aspects. While there is vast literature on perfect and maximum matchings (see, for example, monographs [24] and [4]), the results about maximal matchings are few and scattered through the literature. We mention here two papers that treat, among other topics, maximal matchings in trees [23, 28], one concerned with the structure of equimatchable graphs [17], and a recent paper by the present authors about saturation numbers of benzenoid graphs [11].

Maximal matchings can serve as models of several physical and technical problems such as the block-allocation of a sequential resource or adsorption of dimers on a structured substrate or a molecule. When that process is random, it is clear that the substrate can become saturated by a number of dimers much smaller than the theoretical maximum. The cardinality of any smallest maximal matching in G is the **saturation number** of G. The saturation number of a graph G we denote by s(G). (The same term, saturation number, is also used in the literature with a different meaning; we refer the reader to [14] for more information.)

It is easy to see that the saturation number of a graph G is at least one half of the matching number of G, i.e., $s(G) \ge \nu(G)/2$. Hence, the saturation number provides an information on the worst possible case of clogging; it is a measure of how inefficient the adsorption process can be. However, to fully assess its efficiency, we also need to know how likely it is that the substrate gets saturated by a given number of dimers. In order to answer that question, one must study the enumerative aspects of the problem.

The main goal of this paper is to increase the corpus of knowledge about the enumerative aspects of maximal matchings. Specifically, we compute the efficiency of dimer adsorption for several types of one-dimensional substrates by enumerating maximal matchings of various cardinality in the corresponding graphs. We start with structures of low connectivity and explore how the efficiency depends on the structural properties of their basic building blocks. It turns out that already the structures of the lowest connectivity display interesting patterns of behavior. In some cases we provide explicit formulas for the number of maximal matchings of a given cardinality, while in other cases we establish the recurrences for the enumerating sequences and then use their uni- and bivariate generating functions to determine their asymptotic behavior. Along the way we make several digressions and consider also some graphs that do not fit the above pattern but are amenable to the same approach. We also explore the connections with other combinatorial structures counted by the same enumerating sequences and provide bijective correspondences when possible.

The paper is organized as follows. In the next section we introduce the maximal matching polynomial and list its basic properties. Section 3 is concerned with enumeration of maximal matchings in the simplest linear polymers, the paths and cycles. Section 4 considers the case when basic building blocs are the cycles of length 3 and 4, enumerating maximal matchings in uniform chain cacti. Section 5 moves on to some linear chains of connectivity 2, such as the ladder graphs. (The graphs of sections 4 and 5 belong to the class of fasciagraphs [21].) In section 6 we use the theory of maximal matching polynomials to obtain general results for some classes of thorny graphs, while in section 7 we consider some composite graphs that arise from simpler components *via* two binary operations, the join and the corona product. Finally, in the concluding section we discuss some open problems and indicate some directions of possible future research.

2 Maximal matching polynomial

Matching polynomials are generating functions for the sequences enumerating matchings in a graph G by their size. There are several forms, the two most common being the matching defect polynomial and the matching generating polynomials. Both forms appear as special cases of general matching polynomials introduced by Farrell in [13]. Fortunately, the two forms are closely related and can be used interchangeably. Throughout this paper we prefer the second form.

Let $\Phi_k(G)$ denote the number of matchings in G of size k. The **matching generating** polynomial (or simply the **matching polynomial**) of G is then defined as

$$g(G;x) = \sum_{k=0}^{\nu(G)} \Phi_k(G) x^k.$$

Clearly, g(G; 1) is equal to the total number of matchings in G; this quantity is also known as **Hosoya index** of G and denoted by Z(G). For bipartite graphs, g(G; x) is also known as the **rook polynomial** [25]. We refer the reader to Section 8.5 of [24] for more information on matching polynomials and relationships among them.

The following two properties, together with the fact $g(K_1; x) = 1$, allow us to compute the matching polynomial of any graph by recursively reducing it to trivial components. Here G - e denotes the result of deleting an edge from G but keeping its end-vertices, while $G \setminus e$ denotes the graph obtained from G by deleting both end-vertices of e and all edges incident with them.

Proposition 2.1. Let G be a graph and e an edge of G. Then

$$g(G;x) = g(G - e;x) + x \cdot g(G \setminus e;x).$$

Proposition 2.2. Let G be a graph with components G_1, \ldots, G_k . Then

$$g(G;x) = g(G_1;x) \cdot \ldots \cdot g(G_k;x).$$

By repeated applications of these results one can obtain a recurrence in terms of vertices and their neighborhoods [24].

Proposition 2.3. Let $N(u) = \{v_1, \ldots, v_k\}$ be the neighborhood of a vertex u of G. Then

$$g(G;x) = g(G-u;x) + x \sum_{i=1}^{k} g(G-u-v_i;x).$$

Here the first term accounts for the matching that do not cover u, while the sum counts those covering it.

Let P_n and C_n denote the path and the cycle of length n, respectively. Their matching polynomials are given by following formulas:

$$g(P_n; x) = \sum_{k=0}^{\lfloor n/2 \rfloor} \binom{n+1-k}{k} x^k;$$
$$g(C_n; x) = \sum_{k=0}^{\lfloor n/2 \rfloor} \frac{n}{n-k} \binom{n-k}{k} x^k.$$

From them it follows that the total numbers of matchings in P_n and C_n are given by the Fibonacci and Lucas numbers F_{n+2} and L_n , respectively. Matching polynomials of paths and cycles are closely related to Fibonacci and Lucas polynomials, respectively. The **Fibonacci polynomials** are defined recursively by $f_0(x) = 0$, $f_1(x) = 1$, $f_2(x) = x$ and

$$f_n(x) = x f_{n-1}(x) + f_{n-2}(x)$$

for $n \ge 3$. The Lucas polynomials $\ell_n(x)$ satisfy the same recurrence, but with the initial conditions $\ell_0(x) = 2$, $\ell_1(x) = x$. Evaluated at x = 1 they give the Fibonacci and Lucas numbers, respectively. The following result can be easily verified by direct computation.

Proposition 2.4.

$$f_{n+2}(x) = x^{n+1}g(P_n; x^{-2})$$
 and $\ell_n(x) = x^n g(C_n; x^{-2}).$

Motivated by wide applicability of matching polynomials, we consider the generating function for the sequence counting maximal matchings in a graph G. Let $\Psi_k(G)$ denote the number of maximal matchings of size k in G. The **maximal matching polynomial** of G is defined as

$$m(G;x) = \sum_{k=s(G)}^{\nu(G)} \Psi_k(G) x^k.$$

For example, $m(P_3; x) = x + x^2$, since P_3 contains one maximal matching of size one (the middle edge) and one of size two (covering the vertices of degree one). From the next two examples, $m(C_3; x) = 3x$ and $m(S_3; x) = 3x$ (where S_3 denotes the star $K_{1,3}$), one can see that graphs are not, in general, determined by their maximal matching polynomials. Some further examples are collected in the following proposition. **Proposition 2.5.** $m(\overline{K_n}; x) = 1;$ $m(S_n; x) = nx;$ $m(K_{2n}; x) = \frac{(2n)!}{n!2^n} x^n;$ $m(K_{n,n}; x) = n!x^n;$ $m(K_{m,n}; x) = n^{\underline{m}} x^m \text{ for } m \le n.$

Proof. The first claim is obvious, since there is only one possible matching (the empty one) in a graph without edges. The second claim is also obvious. The next two follow by noticing that in K_{2n} and $K_{n,n}$ every matching can be extended to a perfect matching [24] and plugging in the expressions for the number of perfect matchings in each case. Finally, the fifth claim follows from the fact that the first edge of any matching in $K_{m,n}$ can be chosen in n ways, the second one in n - 1 ways and so on. The process ends when there are no more unsaturated vertices in the smaller class of bipartition. (Here $n^{\underline{m}}$ denotes the falling factorial.)

Let us look at the information encoded in maximal matching polynomials. Its degree is equal to the matching number $\nu(G)$. The lowest degree of x is equal to the saturation number. From there it follows that zero is a root of the maximal matching polynomial of every non-empty graph, and its multiplicity is equal to the saturation number. The set of all powers that appear in m(G; x) is called the **maximal matching spectrum** of G. We denote it by $\sigma_m(G)$. A graph G is **equimatchable** if each maximal matching in G is also a maximum matching [24]. Clearly, a graph G is equimatchable if and only if its maximal matching spectrum is a singleton.

Proposition 2.6. Maximal matching spectrum of any graph G is a set of consecutive nonnegative integers.

Proof. If G is an equimatchable graph, the claim is obviously valid. If G is not an equimatchable graph, then $s(G) < \nu(G)$. We show that for each nonnegative integer $s(G) \leq k \leq \nu(G)$ there exist a maximal matching in G of size k. If k = s(G) or $k = \nu(G)$ the claim is trivially valid. Let now $k < \nu(G)$ and let M be a maximal matching in G of size k. (Such a matching surely exists; at least there is a maximal matching whose size is equal to s(G).) As M is not a maximum matching, there is an M-augmenting path P connecting two vertices not covered by M whose terminal edges are not in M (Theorem 1.2.1 of [24]). The edges of P alternate with respect to M. By switching the edges along this path one obtains matching M' of size k + 1, and M' is also maximal. Hence, for any k between s(G) and $\nu(G)$ there is a maximal matching in G of size k.

Corollary 2.7. Let G be a nontrivial graph. Then

$$\sigma_m(G) = \mathbb{N} \cap [s(G), \nu(G)].$$

Corollary 2.8. The sequence of coefficients of the maximal matching polynomial of a graph G contains no internal zeros.

The maximal matching polynomials share a number of properties with the matching polynomials. For example, Proposition 2.2 is valid also for maximal matching polynomials. However, there is a crucial difference. While the recurrences for matching polynomials are

local, those for the maximal matching polynomials are not. The non-locality means that there is no result for maximal matching polynomials analogous to Proposition 2.1, since we cannot split the set of all maximal matchings into those containing an edge e and those not containing it, without taking into account the edge-neighborhood of e. Similarly, no result analogous to Proposition 2.3 can be stated for maximal matching polynomials of general graphs. This non-locality is the main source of the difficulties while trying to count maximal matchings.

There are, however, classes of graphs in which the edge- and vertex-neighborhoods lead to recurrent relations only a bit more complicated than those for ordinary matching polynomials. As a rule, such graphs are of low connectivity and/or contain vertices of degree one. The fact that (the unique) neighbor of a pendent vertex must be covered by an edge of every maximal matching gives us an analogue of Proposition 2.3. For a given vertex $u \in V(G)$ we denote by $N_1(u)$ the set of all its neighbors of degree one.

Proposition 2.9. Let G be a simple connected graph and $u \in V(G)$ its vertex such that $|N_1(u)| = t > 0$. Then

$$m(G;x) = tx \cdot m(G-u;x) + x \sum_{v \in N(u) \setminus N_1(u)} m(G-u-v;x).$$

Proof. Vertex u must be covered by an edge in each maximal matching of G. It can be one of t pendent edges, in which case the remaining edges must form a valid maximal matching in G - u, or it can be one of the remaining edges incident to u, say uv, in which case the remaining edges must form a maximal matching in G - u - v. In both cases, the size of the maximal matching formed by the remaining edges is one less than the size of matching that covers u, hence the factor x in both terms.

We know that the generating matching polynomials are log-concave [18, 19]. It would be interesting to know if this property is also valid for maximal matching polynomials.

We will make frequent use of the above results in the following sections.

3 Paths and cycles

We remind the reader that throughout this paper P_n denotes the path of length n, hence on n + 1 vertices. As a motivating example, we consider a parking lot made of n + 1 parallel concrete strips such that a car can be parked on any two neighboring strips, as shown in Fig. 1. In ideal situation, when all drivers park responsibly, the lot can accommodate



Figure 1: A parking lot with two parked cars.

 $\lceil n/2 \rceil$ cars. However, if the drivers are careless and park randomly, the lot can become

saturated by a smaller number of cars, as shown in Fig. 2. In the worst possible case, it can become saturated by $\lceil n/3 \rceil$ cars. The problem can be naturally interpreted as a problem of



Figure 2: A saturated parking lot and the corresponding maximal matching.

maximal matching in P_n , as shown in Fig 2. In order to determine the expected number of cars under the random regime of parking, we need to count the number of maximal matching of different sizes in P_n .

We start by counting all maximal matchings in P_n . Let ψ_n denote the total number of maximal matchings in P_n .

Proposition 3.1. The sequence ψ_n is given by the recurrence

$$\psi_n = \psi_{n-2} + \psi_{n-3}$$

for $n \geq 3$. The initial conditions are $\psi_0 = \psi_1 = 1, \psi_2 = 2$.

Proof. Let us label the vertices of P_n by v_0, v_1, \ldots, v_n . Then any maximal matching in P_n must cover v_{n-1} . Those covering it by the edge $v_{n-1}v_n$ are counted by ψ_{n-2} ; those covering it by $v_{n-2}v_{n-1}$ are counted by ψ_{n-3} . The initial conditions are verified by direct computation.

The sequence (ψ_n) is known as the **Padovan sequence**. It appears (shifted by 6) as A000931 in the On-line Encyclopedia of Integer Sequences [26] (in the rest of this paper simply the OEIS). The number of maximal matchings in paths is not mentioned among some seventeen combinatorial interpretations listed there. Hence, we have provided a new combinatorial representation of the Padovan sequence. It would be interesting to provide explicit bijections between maximal matchings in paths and some combinatorial structures listed in the OEIS entry.

Let $\psi_{n,k}$ denote the number of maximal matchings in P_n of size k. It is clear that $\psi_{n,k} = 0$ for too small or too large k. By the same reasoning as in Proposition 3.1 we can prove the recurrence for $\psi_{n,k}$.

Proposition 3.2.

$$\psi_{n,k} = \psi_{n-2,k-1} + \psi_{n-3,k-1}$$

for $n \ge 3$, with the initial conditions $\psi_{0,0} = 1$, $\psi_{1,0} = 0$, $\psi_{1,1} = 1$, $\psi_{2,0} = 0$, $\psi_{2,1} = 2$.

Now we can proceed and obtain the bivariate generating function $\Psi(x, y)$ for $\psi_{n,k}$. We omit the computational details.

Proposition 3.3.

$$\Psi(x,y) = \sum_{n\geq 0} \sum_{k\geq 0} \psi_{n,k} x^n y^k = \frac{1+xy+x^2y}{1-x^2y-x^3y}.$$

The ordinary generating function $\Psi(x) = \sum_{n \geq 0} \psi_n x^n$ is now obtained as

$$\Psi(x) = \Psi(x, 1) = \frac{1 + x + x^2}{1 - x^2 - x^3}$$

Now we employ a variant of Darboux theorem to extract the information about the asymptotic behavior of ψ_n [2]: If the generating function $f(x) = \sum_{n\geq 0} a_n x^n$ of a sequence (a_n) can be written in the form $f(x) = (1 - \frac{x}{w})^{\alpha} h(x)$, where w is the smallest modulus singularity of f and h is analytic in w, then $a_n \sim \frac{h(w)n^{-\alpha-1}}{\Gamma(-\alpha)w^n}$, where Γ denotes the gamma function.

By a straightforward computation we find the smallest modulus singularity of $\Psi(x)$ as the only real solution of $1 - x^2 - x^3 = 0$:

$$w = \frac{1}{6} \left(-2 + (100 - 12\sqrt{69})^{1/3} + (100 + 12\sqrt{69})^{1/3} \right) \approx 0.754878.$$

Its reciprocal value, $1/w \approx 1.324718$, is known as the **plastic constant** [15]. From there we obtain the asymptotics for ψ_n .

Proposition 3.4.

$$\psi_n \sim g(w)w^{-n} = 0.956611 \cdot 1.324718^n.$$

Using the same apparatus we can also compute the expected size of a maximal matching in P_n . Let us denote it by $\pi(P_n)$. It can be computed as

$$\pi(P_n) = \frac{[x^n]\frac{\partial\Psi(x,y)}{\partial y}|_{y=1}}{[x^n]\Psi(x,y)|_{y=1}},$$

where $[x^n]F(x)$ denotes the coefficient of x^n in the expansion of F(x). We omit the computational details and present only the final result.

Proposition 3.5. The expected size of a maximal matching in P_n is given by $\pi(P_n) \approx 0.41149559n$.

Now we define the **efficiency** $\varepsilon(G)$ of random parking on a graph G as the ratio of the expected size of a maximal matching in G and its matching number (the ideal case). Hence, $\varepsilon(G) = \frac{\pi(G)}{\nu(G)}$. In our case,

$$\varepsilon(P_n) = \frac{\pi(P_n)}{\left\lceil \frac{n}{2} \right\rceil}.$$

For large values of n this quantity behaves as $2\pi(P_n) \approx 0.823$. Hence, one can expect that random (or careless) parking will result in using about 82.3% of the full capacity of a linear parking lot.

We could now use the bivariate generating function $\Psi(x, y)$ to obtain closed formulas for the numbers $\psi_{n,k}$. Instead, we provide a combinatorial proof.

Proposition 3.6.

$$\psi_{n,k} = \binom{k+1}{3k-n}.$$

Proof. We use the formula for balls and boxes in the table of the Twelvefold Way at p. 33 in [27]. The balls are the edges participating in a maximal matching, the boxes are defined by the unmatched vertices. There are k edges and n + 1 - 2k unmatched vertices. They define n - 2k + 2 boxes, n - 2k between two vertices and additional 2, one to the left of the leftmost unmatched vertex, the other one to the right of the rightmost one. Into each of n - 2k internal boxes we place one ball (since the unmatched vertices cannot be adjacent). The remaining 3k - n balls can be distributed at will among all n - 2k + 2 boxes. As the number of ways to place a identical balls into b distinct boxes is equal to $\binom{a+b-1}{a}$, the claim follows by using the symmetry property of binomial coefficients.

As usual, we assume that a binomial coefficient is equal to zero if its lower index exceeds the upper one or becomes negative.

Corollary 3.7. The maximal matching polynomial of P_n is given by

$$m(P_n; x) = \sum_{\lceil n/3 \rceil}^{\lceil n/2 \rceil} \binom{k+1}{3k-n} x^n.$$

Corollary 3.8.

$$\psi_n = \sum_{\lceil n/3 \rceil}^{\lceil n/2 \rceil} \binom{k+1}{3k-n}.$$

 \square

The last result gives us the decomposition of Padovan numbers similar to the familiar expression for the Fibonacci numbers, $F_n = \sum_{k\geq 0} \binom{n-k}{k}$. The maximal matching polynomials of P_n satisfy the recurrence $m(P_n; x) = x(m(P_{n-2}; x) + m(P_{n-3}; x))$. Evaluated at x = 1, they give the Padovan numbers. Hence, one could be tempted to call them **Padovan polynomials**. However, the name is already used for another family of polynomials satisfying the recurrence $p_n(x) = xp_{n-2}(x) + p_{n-3}(x)$ with initial conditions $p_1(x) = 1$, $p_2(x) = 0$ and $p_3(x) = x$. It would be interesting to explore our version of Padovan polynomials. We do not know if the expression of Corollary 3.8 is new, but it does not appear in the OEIS.

Before we move to the cycles, we mention that a similar problem was considered in the context of polymerization of organic molecules. Jackson and Montroll [20] used probabilistic reasoning and obtained the value of 0.177 for the average fraction of free radicals in a polymer chain, the same value as the expected fraction of wasted space in our parking lot model. The dynamic aspect of the process was studied by Flory [16], who obtained a slightly larger value of 86.47% (the exact value is $1 - e^{-2}$) for a quantity that we call the efficiency. The difference indicates that some of the most unfavorable configurations are quite unlikely to arise during the process. More information on various models of random and cooperative sequential adsorption can be found in a survey by Evans [12].

Let us now consider the number of maximal matchings in a cycle C_n of length $n \ge 3$. We denote it by φ_n , and the number of maximal matchings in C_n of size k by $\varphi_{n,k}$.

Proposition 3.9. The numbers $\varphi_{n,k}$ are given by the recurrence

$$\varphi_{n,k} = \varphi_{n-2,k-1} + \varphi_{n-3,k-1}$$

for $n \ge 3$, $k \ge 2$, with the initial conditions $\varphi_{0,0} = 3$, $\varphi_{1,0} = \varphi_{1,1} = \varphi_{2,0} = 0$, $\varphi_{2,1} = 2$. The closed form expression is

$$\varphi_{n,k} = \frac{n}{k} \binom{k}{n-2k}.$$

Proof. Let us first consider a cycle C_n for $n \ge 6$. A vertex, say n, can be covered by an edge of a maximal matching of size k in two ways; in each case, the rest of the considered maximal matching must be a maximal matching of size k - 1 in P_{n-3} . If a vertex is not covered by an edge, then both of its neighbors must be covered, and the rest must be a maximal matching of size k - 2 in P_{n-6} . Hence, $\varphi_{n,k} = 2\psi_{n-3,k-1} + \psi_{n-6,k-2}$. The recurrence now follows by plugging in expressions for $\psi_{n,k}$. It can be checked by direct computation that the recurrence remains valid also for n = 3, 4, 5, and the initial conditions are then computed by extending the recurrence backwards to n = 0. The formula follows by taking into account the formula for $\psi_{n,k}$.

The sequence $\varphi_n = \sum_k \varphi_{n,k}$ satisfies the same recurrence as ψ_n , but with different initial conditions, $\varphi_0 = 3$, $\varphi_1 = 0$ and $\varphi_2 = 2$. It is known as the sequence of **Perrin numbers**, and it appears as A001608 in the OEIS. It has the same asymptotics as the Padovan sequence and it can be shown by the same methods we used for paths that the expected size of a maximal matching (and hence the efficiency) in C_n is the same as for the path of the same length. We omit the details.

From Proposition 3.9 we can derive an expression for Perrin numbers in terms of binomial coefficients similar to the expression for Lucas numbers. Again, it is not listed in the OEIS entry.

Corollary 3.10.

$$\varphi_n = \sum_{k \ge 0} \frac{n}{k} \binom{k}{n-2k}$$

4 3- and 4- uniform chain cacti

A **cactus** is a connected graph in which any block is an edge or a cycle. If all blocks of a cactus G are cycles of the same size, say k, we say that G is a k-uniform cactus. In

this section we consider 3- and 4-uniform cacti in which each block has at most two cutvertices, and each cut-vertex is shared by exactly two blocks. Such cacti are called **cactus chains** or **chain cacti**. The number of blocks is the **length** of the chain. Obviously, trees are uniform cacti, all their blocks being copies of K_2 , and paths fit our definitions as the simplest possible cactus chains. This fact lies behind our decision to denote by n the length of P_n and not the number of vertices.

All cactus chains of length n have n-1 cut-vertices. Also, every cactus chain of length n has exactly two blocks with only one cut-vertex. Such blocks are called **terminal**; the remaining (if any) blocks are **internal**. We consider here the cactus chains whose blocks are either triangles or squares. Our goal is to investigate how the richer block structure imposed on the same connectivity pattern affects the number of maximal matchings in such graphs. For both classes we determine the recurrences satisfied by the sequences enumerating maximal matchings of a given size and by the sequence enumerating the total number of maximal matchings. From there we proceed to determine the asymptotics, the expected size and the efficiency using the generating functions in much the same way as in the previous section. We omit most computational details.

4.1 3-uniform cactus chains

It is easy to see that all 3-uniform cactus chains of the same length are isomorphic. Hence we denote such a chain of length n by T_n ; an example is shown in Fig. 3. We will also need auxiliary graphs T'_n such as shown in Fig. 4. The number of maximal matchings in them



Figure 3: A 3-uniform cactus chain.



Figure 4: Auxiliary chain for 3-uniform cactus chains.

we denote by t_n and t'_n , respectively; where $t_{n,k}$ and $t'_{n,k}$ appear, they denote the number of maximal matchings of size k in T_n and T'_n , respectively.

Graph T_n has an odd number of vertices. Hence, it cannot have a perfect matching. It has, however, near-perfect matchings, i.e., matchings that saturate all vertices except one. In fact, $T_n - v$ has a perfect matching for each $v \in V(T_n)$. Graphs with this property are called **factor-critical** graphs. Hence, $\nu(T_n) = n$. The saturation number of T_n is given by $s(T_n) = \lceil \frac{n+1}{2} \rceil$. The claim follows by noticing that any matching of smaller size leaves at least n + 1 vertices uncovered, and at least two of them must belong to the same triangle.

Let us look at the rightmost downward edge in T_n . Each maximal matching of size k must cover at least one of its end-vertices. Those that cover both its end-vertices are counted by $t_{n-1,k-1}$; those that cover only one are counted by $2t'_{n-2,k-1}$. Hence, $t_{n,k} = t_{n-1,k-1} + 2t'_{n-2,k-1}$. Now look at the pending edge of T'_n . Every maximal matching of size k must cover at least one if its end-vertices. Those that cover both are counted by $t'_{n-1,k-1}$; those that cover the cut-vertex by the horizontal edge are counted by $t'_{n-2,k-1}$, and those that cover the cut-vertex by the downward edge are counted by $t_{n-1,k-1}$. Hence, $t'_{n,k} = t'_{n-1,k-1} + t'_{n-2,k-1} + t_{n-1,k-1}$. From there, we can express $t_{n,k}$ as $t_{n,k} = t'_{n+1,k+1} - t'_{n,k} - t'_{n-1,k}$ and obtain a recurrence for $t'_{n,k}$. Once we have the recurrence, we compute the bivariate generating function for $t'_{n,k}$. We leave out the details and state only the final result.

Proposition 4.1.

$$T(x,y) = \sum_{n \ge 0} \sum_{k \ge 0} t_{n,k} x^n y^k = \frac{1 + xy - x^2 y}{1 - 2xy + x^2 y(y-1) - x^3 y^2}.$$

Corollary 4.2.

$$T(x) = \sum_{x \ge 0} t_n x^n = \frac{1 + x - x^2}{1 - 2x - x^3}.$$

Corollary 4.3. The sequence t_n satisfies the recurrence

$$t_n = 2t_{n-1} + t_{n-3}$$

with the initial conditions $t_0 = 1$, $t_1 = 3$ and $t_2 = 5$.

Corollary 4.4. The asymptotic behavior of t_n is given by $t_n \sim 2.205569^n$.

Sequence t_n does not appear in the OEIS. However, the closely related sequence t'_n that satisfies the same recurrence and initial conditions except for $t'_2 = 7$ instead of $t_2 = 5$, is there as the entry A193641. It counts the words of length n over the alphabet $\{0, 1, -1\}$ such that each letter appears in a subsequence of length 2 with the sum zero. We were unable to find a neat bijective correspondence between such words and maximal matchings in T'_n .

When one tabulates $t_{n,k}$ as a triangular array, on its main diagonal appear the numbers of **maximum matchings** in T_n . The following result can be derived from the fact that T_n is factor-critical and that all its blocks are odd cycles. It has been established in a recent paper [9] that such graphs have the minimum possible number of maximum matchings and that this number is equal to the number of vertices.

Proposition 4.5.

$$t_{n,n} = 2n + 1.$$

 \square

We close the subsection by stating the result about the efficiency on 3-uniform cactus chains.

Corollary 4.6.

$$\varepsilon(T_n) \approx 0.74817n.$$

From the above results we can conclude that the additional structure present in the blocks of T_n does not complicate the recurrences - they remain of length 3. The structural enrichment is reflected, though, in the asymptotic behavior of the number of maximal matchings, a consequence of the increased difference between the matching number and the saturation number. Even when the asymptotic behavior is adjusted and expressed in terms of the number of vertices p, $t_n = t_{(p-1)/2} \sim 2.20557^{(p-1)/2} \sim 1.48512^p$, the resulting constant 1.48512 is larger than for P_n . Another consequence is a smaller efficiency, reflecting the fact that in a graph with richer structure of blocks and the same connectivity pattern there are more ways for things to go wrong, i.e., to achieve saturation by a smaller number of dimers.

4.2 4-uniform cactus chains

Unlike their 3-uniform counterparts, the 4-uniform chains of a given length are not all isomorphic. In order to distinguish between various cases, we introduce some terminology borrowed from the benzenoid graphs and 6-uniform cactus chains [8].

Let us look at an internal cycle of a 4-uniform chain. If its two cut-vertices are adjacent, we say that this cycle is an **ortho-cycle**; if the cut-vertices are not adjacent, the cycle is a **para-cycle**. If all internal cycles are of the same type, say, ortho, we call such chain an **ortho-chain** and denote it by O_n ; if all internal cycles are para-cycles, we call the chain a **para-chain** and denote it by Q_n . As in the previous subsection, we leave out routine computations and present only the results. The case of para-chains is simpler and we consider it first.

4.2.1 Para-chains

Let $q_{n,k}$ denote the number of all maximal matchings of size k in Q_n , and q_n the total number of maximal matchings in Q_n . An example is shown in Fig 5. It turns out that those



Figure 5: A para chain of length *n*.

sequences satisfy simpler, i.e., shorter recurrences than sequences t_n and ψ_n . In order to find the recurrences one needs to consider also the auxiliary chains shown in Fig. 6. As before, we omit the details.



Figure 6: Auxiliary graph for para chains.

Proposition 4.7. The bivariate generating function Q(x, y) for the sequence $q_{n,k}$ is given by

$$Q(x,y) = \frac{2xy^2}{1 - 4xy + 2(xy)^2}.$$

Several results now follow as corollaries.

Corollary 4.8. The sequence q_n satisfies the recurrence $q_n = 4q_{n-1} - 2q_{n-2}$ with the initial conditions $q_0 = 0, q_1 = 2$. Its generating function Q(x) is given by $Q(x) = \frac{2x}{1-4x+2x^2}$.

Corollary 4.9.

$$q_n = \frac{(2+\sqrt{2})^n}{\sqrt{2}} - \frac{(2-\sqrt{2})^n}{\sqrt{2}}.$$

The sequence q_n provides a new combinatorial interpretation of sequence A060995 from the OEIS. It counts, among other things, a number of routes of length 2n on the sides of an octagon from a point to opposite point. It would be interesting to provide explicit bijection between such routes and our maximal matchings. It could be also worthwhile to explore its connections with the closely related sequence A007070.

Corollary 4.10. Graph Q_n is equimatchable. Its matching number is equal to n + 1, and its maximal matching polynomial is given by $m(Q_n; x) = q_n x^{n+1}$.

The above result follows from the bivariate generating function,

$$Q(x,y) = 2xy^2 \left(1 + 4(xy) + 14(xy)^2 + 48(xy)^3 + \ldots \right).$$

Another way to derive it is to observe that each cut-vertex must be saturated by an edge of a maximal matching, and that no edge can saturate more that one cut-vertex. That gives us n-1 edges in a maximal matching and the remaining two can be chosen one from each of the two terminal cycles. This fact is also responsible for the small length of the recurrence.

4.2.2 Ortho-chains

An example of an ortho-chain is shown in Fig. 7. A moments reflection should suffice to convince the reader that the property of para-chains regarding the saturation of all cutvertices by all maximal matchings is not preserved for ortho-chains. Hence, it is no wonder that the numbers of maximal matchings in them satisfy again a recurrence of length 3. We state here without proof the basic results for the sequence o_n counting all maximal matchings in O_n



Figure 7: An ortho-chain of length n.

Proposition 4.11. The sequence o_n satisfies the recurrence $o_n = 2o_{n-1} + 2o_{n-2} - 2o_{n-3}$ for $n \ge 3$ with the initial conditions $o_0 = 0$, $o_1 = 2$ and $o_2 = 8$. Its generating function is given by $O(x) = \frac{2x+4x^2}{1-2x-2x^2+2x^3}$. Asymptotically, $o_n \sim 0.36779 \cdot 2.48119^n$.

The sequence does not seem to be in the OEIS.

It would be interesting to examine whether the two considered types of chains are extremal among all chains of a given length. Such behavior is confirmed for matchings and independent sets in hexagonal chains [8].

The methods of this section could be successfully applied also to other types of cactus chains, such as the spiro-chains made of hexagons.

5 Linear polymers of connectivity 2

In this section we move to linear polymers of larger connectivity. As expected, the increase in connectivity will result in longer recurrences; in the two considered cases the lengths will be 8 and 5, respectively. Less clear, however, is the connection between the connectivity and efficiency.

The two polymers considered in this section are shown in Fig. 8 and 9, respectively. The first one, R_n , could be also interpreted as the second power of P_{2n+1} . (The second power,



Figure 8: A 2-connected linear polymer with triangular faces.

1	2	3						n
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Figure 9: The ladder graph.

 G^2 , of a graph G is obtained by connecting by an edge each pair of vertices at distance 2 in G.) The second one is the ladder graph L_n , also known as the linear polyomino.

The results of this section were obtained by the same methods as in the previous cases. We state them in the most condensed form, giving only the generating functions and asymptotic behavior. As before, we omit the computational details.

We denote by r_n and l_n the number of maximal matchings in R_n and L_n , respectively.

Proposition 5.1. The generating function R(x) for the sequence r_n is given by

$$R(x) = \frac{1 + 3x + 2x^2 + 2x^3 - x^5 - x^6 - x^7}{1 - x^2 - 2x^3 - x^4 - x^5 + x^6 + x^8}.$$

Asymptotically, $r_n \sim 1.454145 \cdot 1.625957^n$. The efficiency of R_n is given by $\varepsilon(R_n) \approx 0.849$.

Proposition 5.2. The generating function L(x) for the number of maximal matchings in the ladder graph L_n is given by

$$L(x) = \frac{1 + x^2 + x^3 + x^4}{1 - 2x - x^4 - x^5}.$$

Its asymptotic behavior is given by $l_n \sim 1.110879 \cdot 2.147899^n$. The efficiency of L_n is $\varepsilon(L_n) \approx 0.861799$.

One can see that the recurrence length seems to be influenced more by the highest degree than by the cycle length. This is in line with the intuitive feeling that the recurrence length is mostly dependent on the local complexity. It would be interesting to test this assumption by computing the number of maximal matchings in other chains of connectivity two. According to results reported in [10], the number of maximal matchings in linear polyacenes satisfies a recurrence of legth 5, while for fibonacenes and helicenes the length of recurrence is 7.

Results of the above type could be also obtained by using the method of transfer matrices.

6 Thorny graphs

Let G be a graph on n vertices and m edges. For an ordered n-tuple (p_1, \ldots, p_n) of nonnegative integers we construct a **thorny graph** $T^*(G)$ by attaching p_i pendent vertices to vertex v_i of G. When $p_i = p$ for all i we call such graph a p-**bristle graph** and denote it by $T_p(G)$. When $p_i = p - deg(v_i)$, the resulting graph is called p-**thorny graph**. If G is imagined to be the H-deleted graph of an alkane, then the 4-thorny graph $T^*(G)$ is the H-included graph. Thorny graphs were defined by Cayley [3] and later appeared in the chemical literature as plerographs.

One of the simplest cases arises when $G = P_n$. In that case its *p*-bristle graph $T_p(P_n)$ is called a *p*-caterpillar. An example is shown in Fig 10 below.

Proposition 6.1. The number of maximal matchings in $T_p(P_n)$ is equal to the value of the (n+2)-nd Fibonacci polynomial evaluated at p, i.e., $\Psi(T_p(P_n)) = F_{n+2}(p)$.

Proof. For p > 0 it is clear that every vertex of the original P_n must be covered by an edge of a maximal matching. If the vertex n is covered by the edge $v_{n-1}v_n$, the remaining edges of a maximal matching must form a valid maximal matching in $T_p(P_{n-2})$, and hence are



Figure 10: A 3-caterpillar of length n.

counted by $\Psi(T_p(P_{n-2}))$. If v_n is covered by one of p pending edges, the remaining maximal matchings are counted by $p\Psi(T_p(P_{n-1}))$. Hence the number of maximal matchings in $T_p(P_n)$ satisfies the recurrence

$$\Psi(T_p(P_n)) = p\Psi(T_p(P_{n-1})) + \Psi(T_p(P_{n-2}))$$

with initial conditions $\Psi(T_p(P_0)) = p$, $\Psi(T_p(P_1)) = p^2 + 1$. This is the same recurrence with the same initial conditions as the one satisfied by the Fibonacci polynomials, and the claim follows.

We remind the reader that the Fibonacci polynomials are related to matching polynomials of paths. It can be shown that their appearance here as maximal matching polynomials of caterpillars is not a coincidence. Our next result establishes the relationship between maximal matching polynomials of *p*-bristle graphs and matching polynomials of their underlying graphs.

Theorem 6.2. Let p > 0. Then the maximal matching polynomial of a p-bristle graph $T_p(G)$ is given as

$$m(T_p(G); x) = (px)^n g(G; (p^2 x)^{-1}),$$

where g(G; x) is the matching (generating) polynomial of G.

Proof. Each vertex of G must be covered by an edge of a maximal matching in $T_p(G)$, either by an edge of G, or by any of p new edges. Obviously, $\nu(T_p(G)) = n$, and it is achieved when no edge of G participates in a matching of $T_p(G)$. Let M be a maximal matching in $T_p(G)$ of size l, and let k out of those l edges belong to E(G). These k edges form a matching of size k in G, and each such matching can be extended to a maximal matching in $T_p(G)$ in p^{n-2k} different ways. Then l = k + n - 2k = n - k and $\Psi_{n-k}(T_p(G)) = p^{n-2k}\Phi_k(G)$. The maximal matching polynomial of $T_p(G)$ is now given as $m(T_p(G); x) = \sum_{l=s(T_p(G))}^n \Psi_l(T_p(G))x^l$. By switching to summation over k (the number of edges belonging to E(G)) we obtain

$$m(T_p(G);x) = \sum_{k=0}^{\nu(G)} \Psi_{n-k}(T_p(G))x^{n-k} = \sum_{k=0}^{\nu(G)} p^{n-2k} \Phi_k(G)x^{n-k}$$
$$= (px)^n \sum_{k=0}^{\nu(G)} \Phi_k(G)(xp^2)^{-k} = (px)^n g(G;(p^2x)^{-1}).$$

Now the results on the number of maximal matchings in *p*-thorny graphs of cycles and stars follow as corollaries of the above theorem.

Corollary 6.3. Let p > 0. Then the number of maximal matchings in $T_p(C_n)$ is given as the value of the *n*-th Lucas polynomial evaluated at x = p. Hence, $\Psi(T_p(C_n)) = \ell_n(p)$. \Box **Corollary 6.4.** Let S_n denote the star $K_{1,n}$ and p > 0. Then $\Psi(T_p(S_n)) = (n+p^2)p^{n-1}$.

We close the section by another direct consequence of Theorem 6.2.

Corollary 6.5. Let p > 0. Then $T_p(G)$ is equimatchable if and only if G contains no edges.

7 Composite graphs

Many interesting graphs arise from simpler building blocks *via* some binary operations known as graph products. We consider here two such operations, the sum (also known as join) and the corona product, and apply some of the results obtained in previous sections to enumerate maximal matchings in resulting graphs.

7.1 Sum

Let G_1 and G_2 be two graphs with vertex sets $V(G_i)$ and edge sets $E(G_i)$ for i = 1, 2. Their sum is the graph $G_1 + G_2$ on the vertex set $V(G_1) \cup V(G_2)$ and the edge set $E(G_1 + G_2) = E(G_1) \cup E(G_2) \cup \{\{u, v\}; u \in V(G_1), v \in V(G_2)\}$. In other words, we retain all edges of the component graphs and also join every vertex of G_1 to every vertex of G_2 . The sum of two graphs is sometimes called their **join**. We consider here two special cases when one of the graphs is a single vertex and the other one is a path or a cycle. In the first case we obtain the **fan graph** $J_n = K_1 + P_n$, in the second case the well known **wheel graph** on *n* spokes $W_n = K_1 + C_n$. Examples are shown in Fig. 11.



Figure 11: A fan and a wheel of length 6.

Proposition 7.1.

$$\Psi(J_n) = \sum_{k=0}^n \psi_{k-1}\psi_{n-k-1} + \frac{1 - (-1)^n}{2},$$

where ψ_k is the number of maximal matchings in a path of length k for $k \ge 0$ and $\psi_{-1} = 1$.

Proof. Let $n \ge 1$ be odd. Then a maximal matching in J_n is either a perfect matching in P_n , or it contains an edge covering the vertex of K_1 . The first case is counted by the term $\frac{1-(-1)^n}{2}$. In the second case, if the edge connects K_1 to vertex k in P_n , it splits the base path into two paths of lengths k - 1 and n - k - 1. The result follows by summing over k and taking care of border cases. The case of even n follows in the same way.

The above result provides a combinatorial interpretation for the convolution of the Padovan sequence with itself.

Proposition 7.2.

$$\Psi(W_n) = n\psi_{n-2} + (1 + (-1)^n),$$

where ψ_k is the number of maximal matchings in a path of length k.

Proof. As in the previous proposition, for even n a maximal matching in W_n is either one of the two perfect matchings in C_n (counted by the term $(1 + (-1)^n)$, or it contains a spoke. In the second case, the rest must be a valid maximal matching in P_{n-2} , counted by ψ_{n-2} . The case of odd n is simpler, as any of n spokes can cover the central vertex leaving a maximal matching in P_{n-2} .

Neither of the above sequences appears in the OEIS.

It would be interesting to count maximal matchings in sums of two identical graphs, G + G.

7.2 Corona product

For two graphs G_1 and G_2 we define their **corona product** $G_1 \circ G_2$ as the graph obtained by taking $|V(G_1)|$ copies of G_2 and joining each vertex of the *i*-th copy with vertex $v_i \in V(G_1)$. Unlike in the sum, the components enter the corona product in an asymmetric way. For our purpose it is important that no matter what are connectivities of the components, the corona product has the connectivity one. That will allow us to apply the decompositions that worked in previous sections and count maximal matchings in some simple cases. The *p*-bristle graph of the previous section is a corona product of G and $\overline{K_p}$, while $J_n = K_1 \circ P_n$ and $W_n = K_1 \circ C_n$. We consider first the case $P_n \circ P_1 = P_n \circ K_2$.

Proposition 7.3. The sequence $p_n = \Psi(P_n \circ P_1)$ satisfies the recurrence $p_n = 2p_{n-1} + 3p_{n-2} + p_{n-3}$ with the initial conditions $p_0 = 3$, $p_1 = 9$, $p_2 = 28$.

Proof. An example of $P_n \circ P_1$ is shown in Fig. 12 below. Each maximal matching in $P_n \circ P_1$ either covers vertex labeled v_n in P_n or does not cover it. In the first case, the remaining edges must form either a valid matching in $P_{n-1} \circ P_1$ (if v_n is covered by one



Figure 12: $P_n \circ P_1$.

of two edges toward its copy of P_1) or a valid maximal matching in $P_{n-2} \circ P_1$ (if v_n is covered by $v_{n-1}v_n$). There are altogether $2p_{n-1} + p_{n-2}$ maximal matchings covering v_n . Maximal matchings that do not cover v_n must cover v_{n-1} and are counted by the expression of the same type, with indices decreased by one. The claim now follows by adding the two contributions.

The sequence (p_n) appears as A084084 in the OEIS without combinatorial interpretations.

Our last example in this section demonstrates interesting connections between maximal matchings and tilings.

Proposition 7.4.

$$\Psi(P_n \circ K_3) = 3^{n+1} F_{n+2}.$$

Proof. The result follows by the same reasoning as in the previous proposition, but the resulting recurrence is shorter, since each vertex of the backbone P_n must be covered by an edge of any maximal matching. The situation is shown in Fig. 13. Taking into account



Figure 13: Maximal matchings covering v_n in $P_n \circ K_3$.

that there are 3 (maximal) matchings in K_3 we obtain a recurrence of length 2,

$$\Psi(P_n \circ K_3) = 3\Psi(P_{n-1} \circ K_3) + 9\Psi(P_{n-2} \circ K_3).$$

The same recurrence with the same initial conditions is satisfied by the sequence $3^{n+1}F_{n+2}$, hence the claim.

We leave to the reader to show that the sequence $3^{n+1}F_{n+2}$ also counts tilings of a row of n unit squares by unit squares and dominoes such that the squares come in any of 3 colors and the dominoes in any of 9 colors.

The recurrence for the number of maximal matchings in $P_n \circ K_3$ is shorter than the recurrence for a simpler graph $P_n \circ K_2$. That is a consequence of factor-criticality of K_3 . It could be shown that the number of maximal matchings of $P_n \circ G$ satisfies a recurrence of length 2 whenever G is factor-critical.

8 Concluding remarks

The present manuscript is, to the best of our knowledge, the first systematic attempt to address enumerative aspects of maximal matchings. We have counted maximal matchings in several classes of graphs of low connectivity. In most cases, we have obtained complete information, including the generating functions and asymptotic behavior of the enumerating sequences; in some particular cases we were even able to obtain closed formulas. The obtained results are, however, far from comprehensive. In this section we list some open problems and possible directions for future research. One obvious direction is to continue our work on cactus chains. It could be done by considering uniform cacti whose blocks are larger cycles, such as hexagons. With larger cycles comes also greater variability in the connectivity patterns, leading to the problem of finding the extremal chains among all uniform chains of the same length. We left the problem open even for 4-uniform chains.

Another possibility is to look at non-uniform chains. Examples of such chains can be obtained from uniform chains by expanding each cut-vertex into an edge. We have done some preliminary work on this type of chains and noticed that the enumerating sequences also appear in some other combinatorial contexts. Providing explicit bijections among the corresponding families is the goal of our paper currently under preparation.

Among the linear polymers of connectivity 2 the most interesting ones are, without doubt, the benzenoid chains. Some recent findings are reported in [10]. There are indications that the extremality patterns valid for perfect matchings and all matchings do not persist for maximal matchings.

We have addressed here only the composite graphs of low connectivity. However, many interesting operations such as, e.g., the Cartesian product, actually increase the connectivity. It would be probably too ambitious to hope for general enumerative results for Cartesian products, but the cases when one factor is a path or a cycle should not be out of reach. Another interesting thing in such graphs would be their saturation number; at the present, there are only few known results of this type.

Finally, it would be worthwhile to try to develop a general theory of maximal matching polynomials and to see if they could play as important role in the study of maximal matchings as the matching polynomials have played so far in the general context of matchings. In particular, it would be interesting to see if their coefficients form log-concave or unimodal sequences for all graphs.

Acknowledgment This work has been supported in part by Croatian Science Foundation under the project 8481 (BioAmpMode).

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