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Counting Dominating Sets in Cactus Chains

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Abstract. In this paper we consider the number of dominating sets in cactus chains with triangular and square blocks. We derive and solve the recurrences satisfied by those quantities and investigate their asymptotic behavior. In triangular case we also refine the counting by computing the bivariate generating function. As a corollary, we compute the expected size of a dominating set in a triangular cactus chain of a given length.

1. Introduction

A **dominating set** of a graph $G = (V, E)$ is any subset D of V such that every vertex not in D is adjacent to at least one member of D. The **domination number** $\gamma(G)$ is the cardinality of a smallest dominating set in G. The domination number is one of the most thoroughly studied simple graph invariants. Several books ([8, 9]) are written on this invariant alone, and some twenty years ago there were already hundreds of papers concerned with domination in particular classes of graphs [11]. Also, the concept of domination and related invariants have been generalized in many ways. Among the best know generalizations are total, independent, and connected domination, each of them with the corresponding domination number; see [7, 12] for a survey of recent results.

Most of the papers published so far deal with structural aspects of domination, trying to determine exact expressions for $\gamma(G)$ or some upper and/or lower bounds for it. The enumerative side of the problem is not so well researched, although its roots can be traced back to a classical paper by Merrifield and Simmons [17]. There they remarked that they were unable to obtain a recurrence for the number of dominating sets (or the externally stable vertex sets, as they called them) for general graphs. Instead, they provided a Fibonacci-like recurrence for paths and observed that the number of dominating sets seems to be odd for all graphs. Almost thirty years passed before a proof of the observation was published by Brouwer, Csorba and Schrijver [4]. Gradually, a number of papers appeared concerned with enumerating some types of dominating sets in paths and cycles [22] and with an attempt to develop a theory of domination polynomials analogous to the familiar matching and independence polynomials [1, 2]. One of the reasons for the lack of results might be the fact that problems of this type are hard: For example, even in restricted graph classes such as, e.g., split graphs and bipartite chordal graphs, counting the number of dominating

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sets is #P-complete [15]. Hence, it makes sense to look for classes of graphs where this problem can be efficiently solved. As most of the difficulties stem from the fact that the recurrences for the number of dominating sets are "less local" than the recurrences that appear in counting matchings and independent sets, it is natural to look to the classes of graphs with simple connectivity patterns, for example cacti.

The goal of the present paper is to further contribute to the corpus of knowledge about the enumerative aspects of domination by investigating the number of dominating sets in two classes of simple linear polymers called cactus chains. Cactus graphs were first known as Husimi trees; they appeared in the scientific literature some sixty years ago in papers by Husimi and Riddell concerned with cluster integrals in the theory of condensation in statistical mechanics [10, 14, 18]. In the meantime, they also found applications in chemistry [13, 21] and in the theory of electrical and communication networks [20], when it turned out that some computationally difficult problems can be solved on cacti in polynomial time. We refer the reader to papers [5, 16] for some aspects of domination in cactus graphs and to [6] for some enumerative results on matchings and independent sets in chain cacti.

In the rest of the paper we study how the number of dominating sets depends on the connectivity patterns in the chain. For simple connectivity patterns we derive linear recurrences that, in turn, yield explicit formulas and the asymptotics. At the end, we investigate effects of introducing a defect in a chain with a homogeneous connectivity pattern.

2. Definitions and Preliminaries

A **cactus graph** is a connected graph in which no edge lies in more than one cycle. Consequently, each block of a cactus graph is either an edge or a cycle. If all blocks of a cactus G are cycles of the same size m, the cactus is m-**uniform**.

A **triangular cactus** is a graph whose blocks are triangles, i.e., a 3-uniform cactus. A vertex shared by two or more triangles is called a **cut-vertex**. If each triangle of a triangular cactus G has at most two cut-vertices, and each cut-vertex is shared by exactly two triangles, we say that G is a **chain triangular cactus**. The number of triangles in G is called the **length** of the chain. An example of a chain triangular cactus is shown in Fig. 1. Obviously a chain triangular cactus of length n has $2n + 1$ vertices and $3n$ edges.

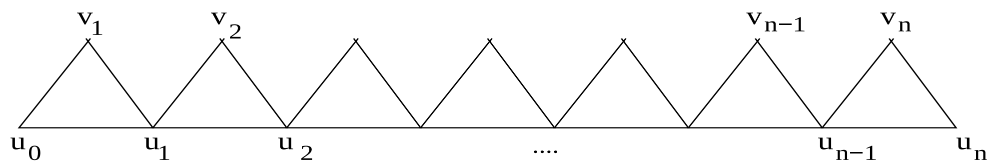

Figure 1: The chain triangular cactus of length 7.

Furthermore, any chain triangular cactus of length greater than one has exactly two triangles with only one cut-vertex. Such triangles are called **terminal triangles**. Any remaining triangles are called **internal triangles**. Obviously, all chain triangular cacti of the same length are isomorphic. Hence, we denote the chain triangular cactus of length n by T_n.

By replacing triangles in the above definitions by cycles of length 4 we obtain cacti whose every block is C_4. We call such cacti **square cacti**. An example of a square cactus chain is shown in Fig. 2. We see that the internal squares may differ in the way they connect to their neighbors. If their cut-vertices are adjacent, we say that such a square is an **ortho-square**; if the cut-vertices are not adjacent, we call the square a **para-square**. (The terminology is borrowed from the theory of benzenoid hydrocarbons; see [6] for more details.) The set of all chain square cacti of length n will be denoted by $\mathcal{S}_n$. The unique square cactus chain of length n whose all internal squares are para-squares we denote by Q_n, while the unique ortho-chain will be denoted by S_n.

Chains T_n and Q_n are among the simplest chain cacti; the only simpler chain cactus is the path P_n, whose all blocks are single edges. Dominating sets in paths were counted in [22] and we refer the reader to this reference for the proof of the following result.

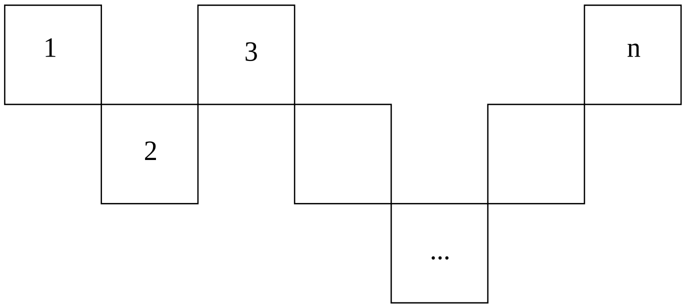

Figure 2: A chain square cactus of length 7.

Theorem A
Let us denote by d_n the number of dominating sets in P_n. Then the numbers d_n satisfy the following recurrence for $n \geq 4$:

$$d_n = d_{n-1} + d_{n-2} + d_{n-3},$$

with the initial conditions $d_1 = 1, d_2 = 3, d_3 = 5$. □

Hence the enumerating sequence for dominating sets in P_n is the (shifted) Tribonacci sequence. Its asymptotic behavior is given by $d_n \sim 1.839286^n$ for large n.

3. Counting Dominating Sets in T_n

Let us consider T_n labeled in the way shown in Fig. 1 and denote the number of dominating sets in T_n by t_n. Each dominating set in T_n either does or does not contain vertex u_n. Let us denote by t'_n the number of dominating sets that contain u_n, and by t''_n the number of dominating sets that do not contain u_n. Hence, $t_n = t'_n + t''_n$. Obviously, $t'_n = 2t_{n-1}$, since each dominating set in T_{n-1} can be extended to a dominating set in T_n counted by t'_n in exactly two ways. Now we consider the dominating sets counted by t''_n. If such a set contains v_n, then each dominating set in T_{n-1} can be extended to a dominating set in T_n counted by t''_n. If such a set does not contain v_n, then it must contain u_{n-1}; if not, then u_n will not be dominated. Such sets are counted by $t'_{n-1} = 2t_{n-2}$. Hence, $t''_n = t_{n-1} + 2t_{n-2}$. Now, from $t_n = t'_n + t''_n$ we obtain the recurrence satisfied by the numbers t_n for $n \geq 3$. The initial conditions $t_1 = 7$ and $t_2 = 25$ are easily verified by direct counting. In fact, the recurrence remains valid even if we start from $t_0 = 2$.

Theorem 1
The enumerating sequence (t_n) for the number of dominating sets in T_n is given by the recurrence

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

for $n \geq 2$ and the initial conditions $t_0 = 2, t_1 = 7$. □

By a routine computation we can now obtain the generating function $T(x) = \sum_{n=0}^{\infty} t_n x^n$ for t_n.

Corollary 2

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

□

Now we can use a version of Darboux theorem to deduce the asymptotic behavior of t_n. We refer the reader to any of standard books on generating functions, such as [3, 19] for more information on these techniques.

Theorem B (Darboux)
Let $f(x) = \sum_{n=0}^{\infty} a_n x^n$ denote the generating function of a sequence (a_n). If $f(x)$ can be written as

$$f(x) = \left(1 - \frac{x}{w}\right)^{\alpha} g(x),$$

where w is the smallest modulus singularity of f and g is analytic at w, then

$$a_n \sim \frac{g(w)}{\Gamma(-\alpha)} w^{-n} n^{-\alpha-1}.$$

Here $\Gamma(x)$ denotes the gamma function. □

Now by a routine computation we obtain the asymptotics for t_n. We omit the details.

Corollary 3

$$t_n \sim \left(1 + \frac{4}{\sqrt{17}}\right)\left(\frac{3+\sqrt{17}}{2}\right)^n.$$

□

Numerically, we have $t_n \sim 1.9701425 \cdot 3.5615528^n$.

Let us now refine our results by decomposing the number of dominating sets in T_n by their cardinality. We denote by $t_{n,k}$ the number of dominating sets in T_n of cardinality k. If a dominating set of cardinality k in T_n contains both of u_n and v_n, then the rest of it is a dominating set of cardinality $k-2$ in T_{n-1}, and there are $t_{n-1,k-2}$ such sets. This is the top case in the middle column in Fig. 3. If such a set contains only u_n or v_n,

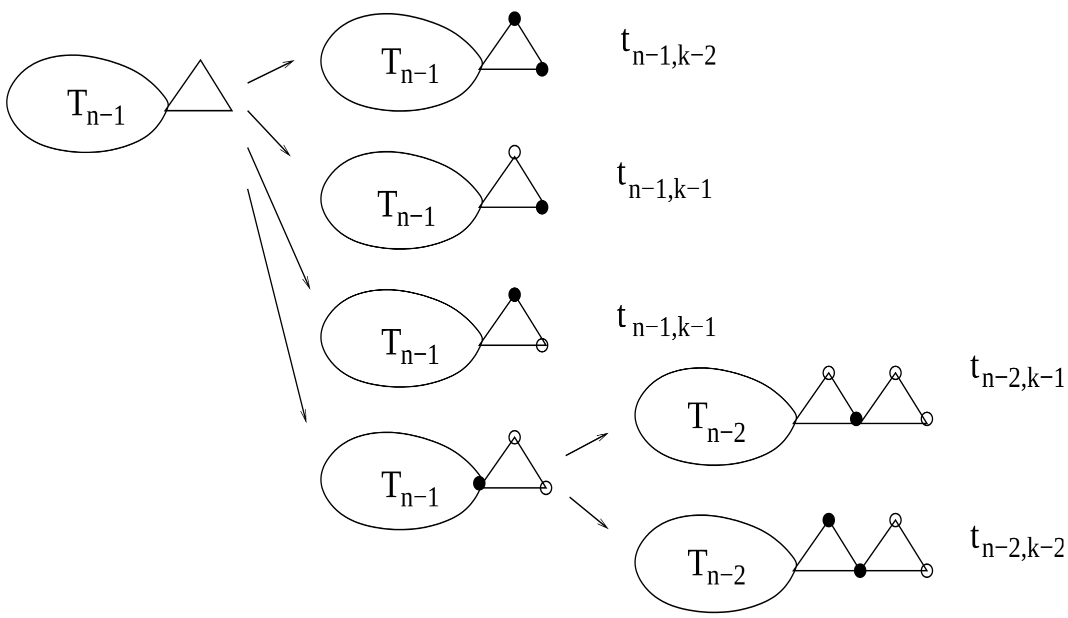

Figure 3: Derivation of the recurrence for $t_{n,k}$.

the rest of it is a dominating set of cardinality $k-1$ in T_{n-1}; such sets are counted by $t_{n-1,k-1}$. Finally, if such a set contains none of u_n and v_n, then we have the situation shown in the right column of Fig. 3. There are two possibilities and they are counted by $t_{n-2,k-1}$ and $t_{n-2,k-2}$, *respectively*. By adding all contributions we obtain the recurrence for $t_{n,k}$. It is valid for $n, k \geq 3$:

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

The initial conditions are again obtained by direct counting.

The bivariate generating function $T(x,y) = \sum_{n,k\geq 0} t_{n,k} x^n y^k$ can be obtained by a routine computation and we omit the details.

Corollary 4

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

□

By computing $\frac{\partial}{\partial y}D(x,y)\Big|_{y=1}$ and finding the asymptotic behavior of its coefficients we can compute the expected size of a dominating set in T_n. Again, we refer the reader to standard books on generating functions and omit the details.

Corollary 5
Let e_n denote the expected size of a dominating set in T_n. Then

$$e_n \sim \frac{3\sqrt{17}+7}{4\sqrt{17}}n \approx 1.174437n.$$

□

Since the domination number of T_n is $\left\lceil \frac{n}{2} \right\rceil$, we see that the average dominating set in T_n is pretty inefficient.

It is interesting to note that the recurrence for t_n is shorter than the recurrence for the numbers d_n from theorem A, although P_n has simpler structure than T_n. It seems that the presence of the vertex v_n prevents the effects of u_n being included or not included from spreading too far down the chain.

Before we leave triangular cacti we mention a graph known as the windmill graph W_n. It is the triangular cactus with n triangles that all share a single cut-vertex. An example is shown in Fig. 4. It is easily seen that the number of dominating sets in W_n is equal to $4^n + 3^n$ for $n \geq 1$. As the vertex set of W_n has $2^{2n+1} = 2 \cdot 4^n$

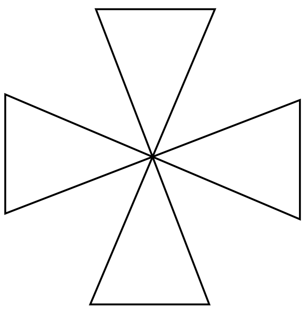

Figure 4: Windmill graph W_4.

subsets, we see that about one half of all subsets are dominating sets, while the proportion of the subsets of vertices of T_n that are also dominating sets is exponentially small, tending to zero as $\left(\frac{3.56155}{4}\right)^n$.

4. Counting Dominating Sets in Chains of Squares

In this section we count dominating sets in two classes of chains with all internal squares of the same type. We start with the para-chain.

4.1. *Para-chain Q_n*

We consider a para-chain of length n, labeled as shown in Fig. 5. The number of dominating sets in Q_n is denoted by q_n. As before, by q'_n we denote the number of dominating sets that contain v_n, and by q''_n the number of dominating sets that do not contain v_n. Again, $q_n = q'_n + q''_n$. In addition, we denote by $\tilde{q}_n$ the number of sets that are not dominating in Q_n but can be extended to a dominating set in Q_{n+1}. Clearly, such sets do not include v_n, but they must include v_{n-1}, since this vertex is necessary to dominate t_n and b_n. Hence, they are counted by q'_{n-1} and we have $\tilde{q}_n = q'_{n-1}$.

Now we find three recurrences for q'_n, q''_n and $\tilde{q}_n$.

Each dominating set in Q_n counted by q'_n can be extended to a dominating set in Q_{n+1} counted by q'_{n+1} in exactly four ways. Further, a dominating set in Q_n counted by q''_n can be extended to a dominating set

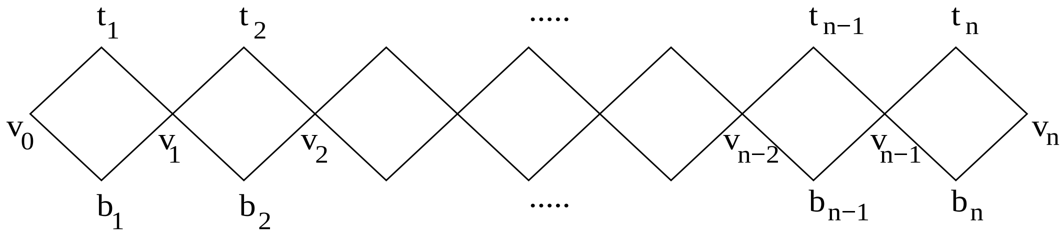

Figure 5: The labeling of para-chain Q_n.

in Q_{n+1} counted by q'_{n+1} also in four ways. Finally, a set counted by $\tilde{q}_n$ can be extended to a dominating set counted by q'_{n+1} in exactly three ways. By adding all contributions we obtain the recurrence for q'_n,

$$q'_{n+1} = 4q'_n + 4q''_n + 3\tilde{q}_n.$$

Now we need a recurrence for q''_n. Each dominating set in Q_n that includes v_n can be extended to a dominating set in Q_{n+1} counted by q''_{n+1} in three ways. Further, a dominating set counted by q''_n can be extended to a dominating set in Q_{n+1} counted by q''_{n+1} in only one way, by including both t_{n+1} and b_{n+1}, and the same is valid for the sets counted by $\tilde{q}_n$. Hence,

$$q''_{n+1} = 3q'_n + q''_n + \tilde{q}_n.$$

Finally, we have shown above that $\tilde{q}_{n+1} = q'_n$, and this is our third recurrence. We have obtained the system

$$\begin{array}{rclcrcrcr} q'_{n+1} & = & 4q'_n & + & 4q''_n & + & 3\tilde{q}_n \\ q''_{n+1} & = & 3q'_n & + & q''_n & + & \tilde{q}_n \\ \tilde{q}_{n+1} & = & q'_n & & & & \end{array}$$

with the initial conditions $q'_1 = 7$, $q''_1 = 4$ and $\tilde{q}_1 = 1$.

Now we introduce three generating functions, $Q'(x) = \sum_{n\geq 0} q'_{n+1}x^n$, $Q''(x) = \sum_{n\geq 0} q''_{n+1}x^n$ and $\tilde{Q}(x) = \sum_{n\geq 0} \tilde{q}_{n+1}x^n$. By multiplying all equations in the above system through by x^n and then summing over all $n \geq 0$, the system can be translated into a linear system for three unknown generating functions:

$$\begin{array}{rcrcrcl} (1-4x)Q'(x) & - & 4xQ''(x) & - & 3x\tilde{Q}(x) & = & 7 \\ -3xQ'(x) & + & (1-x)Q''(x) & - & x\tilde{Q}(x) & = & 4 \\ -xQ'(x) & & & + & \tilde{Q}(x) & = & 1 \end{array}$$

The system can be easily solved by using Cramer rule. We obtain

$$Q'(x) = \frac{7+12x+x^2}{1-5x-11x^2-x^3}, \quad Q''(x) = \frac{4+6x}{1-5x-11x^2-x^3}, \quad \tilde{Q}(x) = \frac{1+2x+x^2}{1-5x-11x^2-x^3}.$$

Finally, by adding $Q'(x)$ and $Q''(x)$ and multiplying the sum by x we obtain the generating function for the sequence (q_n).

Theorem 6

$$Q(x) = \sum_{n=0}^{\infty} q_n x^n = \frac{11x+18x^2+x^3}{1-5x-11x^2-x^3}.$$

□

Since $Q(x)$ is a rational function, we can conclude that the numbers q_n satisfy a third order linear recurrence with constant coefficients. The initial conditions can be verified by direct computations.

Corollary 7

The number q_n of dominating sets in Q_n is given by the recurrence

$$q_n = 5q_{n-1} + 11q_{n-2} + q_{n-3}$$

for $n \geq 4$ with the initial conditions $q_1 = 11$, $q_2 = 73$, and $q_3 = 487$. □

The equation $1 - 5x - 11x^2 - x^3 = 0$ has three real solutions. The smallest modulus one is approximately 0.1498954. Hence, the asymptotic behavior of q_n is given by $q_n \sim 6.671318^{n+1}$ for large n.

4.2. *Ortho-chain S_n*

Now we consider the ortho-chain S_n of length n labeled as shown in Fig. 6. The number of dominating

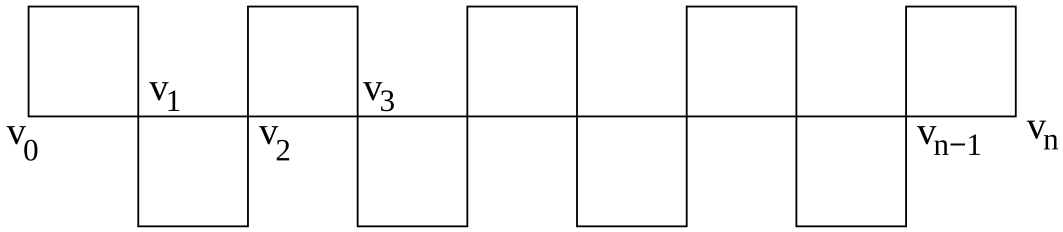

Figure 6: The labeling of ortho-chain S_n.

sets in S_n is denoted by s_n, and the numbers of dominating sets containing and not containing v_n, are denoted by s'_n and s''_n, respectively. Finally, by $\tilde{s}_n$ we denote the number of sets of vertices that are not dominating in S_n, but can be extended to a dominating set in S_{n+1}.

By a reasoning completely analogous to the one employed for para-chains, we obtain the system of recurrences for s'_n, s''_n and $\tilde{s}_n$:

$$\begin{array}{rcrcrcr} s'_{n+1} & = & 4s'_n & + & 3s''_n & + & 3\tilde{s}_n \\ s''_{n+1} & = & 3s'_n & + & 2s''_n & + & \tilde{s}_n \\ \tilde{s}_{n+1} & = & & & s''_n & + & \tilde{s}_n \end{array}$$

with the same initial conditions as for the para-chain. Again, we introduce the corresponding generating functions $S'(x) = \sum_{n\geq 0} s'_{n+1}x^n$, $S''(x) = \sum_{n\geq 0} s''_{n+1}x^n$ and $\tilde{S}(x) = \sum_{n\geq 0} \tilde{s}_{n+1}x^n$ and obtain a linear system for them of the form

$$\begin{array}{rcrcrcl} (1-4x)S'(x) & - & 3xS''(x) & - & 3x\tilde{S}(x) & = & 7 \\ -3xS'(x) & + & (1-2x)S''(x) & - & x\tilde{S}(x) & = & 4 \\ & - & xS''(x) & + & (1-x)\tilde{S}(x) & = & 1 \end{array}$$

Its solution is the triple

$$S'(x) = \frac{7 - 6x + 4x^2}{1 - 7x + 4x^2 - 4x^3}, \quad S''(x) = \frac{4 + 2x}{1 - 7x + 4x^2 - 4x^3}, \quad \tilde{S}(x) = \frac{1 - 2x + 4x^2}{1 - 7x + 4x^2 - 4x^3}.$$

From there we obtain the generating function $S(x)$ of the sequence (s_n).

Theorem 8

$$S(x) = \sum_{n=0}^{\infty} s_n x^n = \frac{11x - 4x^2 + 4x^3}{1 - 7x + 4x^2 - 4x^3}.$$

□

Again, we conclude that the numbers s_n satisfy a third-order linear recurrence with the same coefficients as the polynomial in the denominator of $S(x)$.

Corollary 9

The numbers s_n satisfy the recurrence

$$s_n = 7s_{n-1} - 4s_{n-2} + 4s_{n-3},$$

with the initial conditions $s_1 = 11$, $s_2 = 73$ and $s_3 = 471$. □

The smallest modulus root of equation $1 - 7x + 4x^2 - 4x^3 = 0$ is approximately equal to 0.15437; hence the asymptotic behavior of s_n is given by $s_n \sim 6.47783^{n+1}$. We see that the ortho-chain has fewer dominating sets than the para-chain of the same length.

5. Concluding Remarks

We have investigated here the number of dominating sets in several classes of uniform chain cacti. For the triangular chains the problem is completely solved, since all chains of given length are isomorphic. For square chains, however, some questions remain open. It would be interesting, for example, to show that the para- and the ortho-chain are extremal with respect to the number of dominating sets. As a step in that direction, we will investigate the effect of a single ortho-defect in a para-chain. The situation is shown in Fig. 7. We denote this graph by D_{mn} and the number of dominating sets in it by d_{mn}.

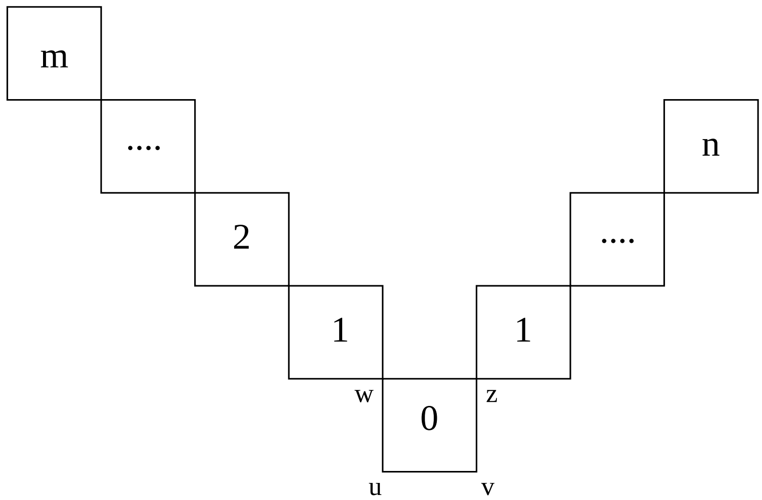

Figure 7: A para-chain with a single ortho-defect.

In order to compute d_{mn}, we must consider four cases: whether a dominating set contains both, one or none of vertices u and v. The case of none is the simplest: if a dominating set in D_{mn} contains none of u, v, then it must contain both of w and z, and there are exactly $q'_m \cdot q'_n$ such dominating sets.

Let us now look at the case when a dominating set in D_{mn} contains u but not v. There are $q'_n(q_m + \tilde{q}_m)$ such sets containing z and $q_m q''_n + q'_m \tilde{q}_n$ such sets that do not contain z. Hence, there are altogether $q_m q_n + q'_n \tilde{q}_m + q'_m \tilde{q}_n$ dominating sets containing u but not v. By symmetry, there must be $q_n q_m + q'_m \tilde{q}_n + q'_n \tilde{q}_m$ dominating sets that contain v but not u. Finally, there are $(q_m + \tilde{q}_m)(q_n + \tilde{q}_n)$ dominating sets in D_{mn} that contain both u and v. By summing the above contributions we obtain the following result:

$$d_{mn} = 3q_m q_n + q'_m q'_n + 2q'_m \tilde{q}_n + 2q'_n \tilde{q}_m + q_m \tilde{q}_n + q_n \tilde{q}_m + \tilde{q}_m \tilde{q}_n.$$

As an example, we take a para-chain of length p and perturb it by introducing a single ortho-defect at place n_d, where $n_d = 1, \dots, p-2$ denotes the position of the ortho-square among internal squares. The ratio r_d defined as $r_d = \frac{d_{mn}}{d_p}$, where $m + n = p - 1$ for $p = 11$ and $p = 21$ is shown in Fig. 8. We see that the effects are strongest for defects near the ends of the chain. It is interesting to observe the role of parity of n_d.

There are also another interesting questions. For example, how the connectivity pattern affects the length of recurrences for the number of dominating sets in m-uniform chains for $m \geq 5$? Finally, it would be interesting to compare the extremality of such chains with the cases of matchings and independent sets [6].

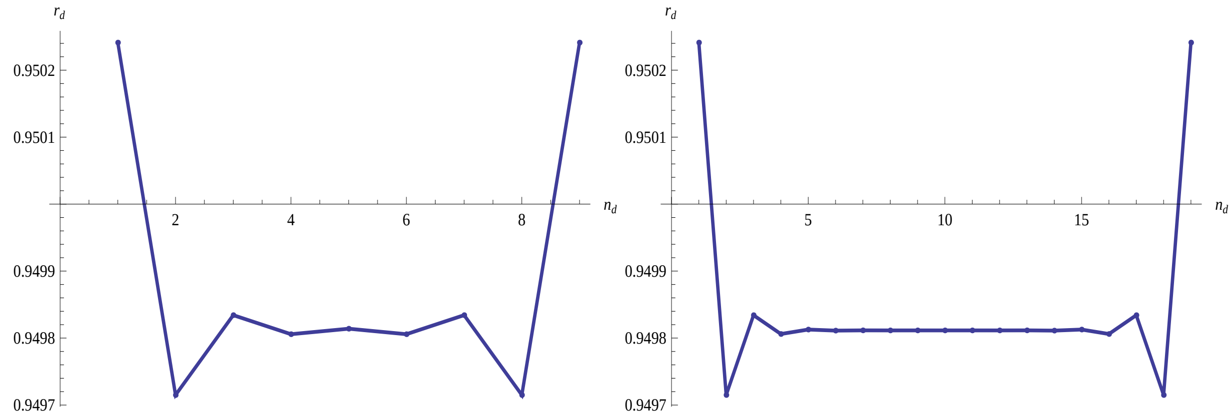

Figure 8: Effects of a single ortho-defect in a para-chain of length 11 (left) and 21 (right).

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