Tomislav Došlić, Ivica Martinjak (Eds.)

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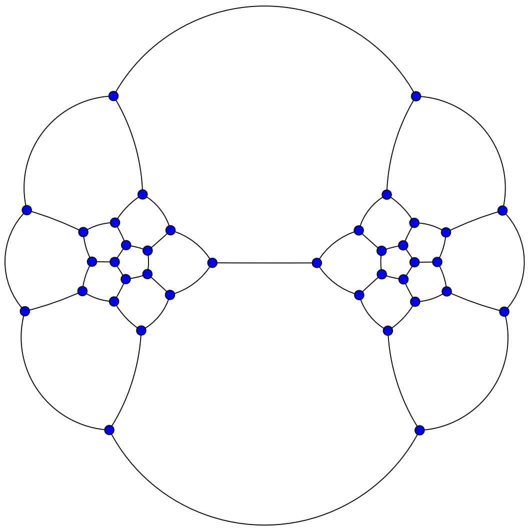

1st Croatian Combinatorial Days

Zagreb, September 29 – 30, 2016

Faculty of Civil Engineering, University of Zagreb

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The cover art is the planar Lombardi drawing of a 38-vertex graph with girth five and cyclic edge connectivity three by David Eppstein (arxiv:1206.6142v1), used with permition of the author.

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Preface

The idea of organizing a gathering of Croatian combinatorialists and discrete mathematicians had been around for several years. We finally decided to give it a try at the margins of the 6^{th} Croatian Mathematical Congress in June of 2016, when we agreed that a rather informal and unpretentious meeting could be organized by the end of September of 2016. The intended informal and relaxed character of the gathering was signalled by the choice of CroCoDays as its working title.

In spite of being organized on a short notice and on a shoestring budget, the meeting succeeded over all expectations. It was attended by over forty participants representing institutions from five countries, and twenty five participants gave oral presentations of their work. We are particularly glad that, besides senior scientists, the meeting also attracted several undergraduate and graduate students, whose participation was made in part possible by a generous subsidy from the Faculty of Civil Engineering.

At first we have not planned publishing the proceedings of our meeting. However, motivated by wide scope and good quality of the talks, we have approached several speakers asking them to write their contributions and submit them for a refereeing process. The present volume is the result. It took us more time and effort than we expected, but we do not regret the decision to publish it. We hope that it will remind the participants on the first CroCoDays and motivate them (and also other readers) to plan attending the next meeting(s).

We thank to all participants of the 1^{st} CroCoDays and to all contributors to this volume. We also thank the reviewers for their help. Particular thanks go to the Faculty of Civil Engineering for providing logistic and financial support for both the meeting and this publication.

Zagreb, November 2017

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On certain families of planar patterns and fractals

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This paper is dedicated to Professor Robert F. Tichy on the occasion of his 60^th anniversary.

Abstract

This survey article is dedicated to some families of fractals that were introduced and studied during the last decade, more precisely, families of Sierpiński carpets: limit net sets, generalised Sierpiński carpets and labyrinth fractals. We give a unifying approach of these fractals and several of their topological and geometrical properties, by using the framework of planar patterns.

Keywords: fractal, Sierpiński carpet, pattern, graph, connectedness, dendrite, path length, arc length

MSC: 28A80, 05C38, 28A75, 51M25, 54D05, 54F50

1.1 Introduction

Sierpiński carpets are self-similar fractals in the plane that originate from the classical Sierpiński carpet [27, 41]. Sierpiński carpets are constructed by dividing the unit square

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into $m \times m$ congruent smaller subsquares of which m_0 squares are cut out together with their boundary, and then taking the closure. The resulting pattern is the *generator* of the Sierpiński carpet. At each step of the iterative construction this procedure is applied to all remaining squares, and, repeating this construction ad infinitum, the resulting object is a fractal of Hausdorff dimension $\frac{\log(m^2-m_0)}{\log(m)}$, called a *Sierpiński carpet* [20]. Figure 5 shows the first two steps of the iterative construction of a Sierpiński carpet.

These fractals can also be defined as attractors of IFS (for Iterated Functions Systems we refer, e.g., to the books of Falconer [18, 19] and Barnsley [3, 4]), and occur in several branches of mathematics. In particular, their geometric and topological properties gained a lot of interest, see, e.g., Whyburn [43], Curtis and Fort [16], McMullen [31], Bandt and Mubarak [1], Lau et al. [25]. During the last decades Sierpiński carpets have been used, e.g., as models for porous materials [20, 42].

Limit net sets, generalised Sierpiński carpets and labyrinth fractals are families of Sierpiński carpets that were introduced and studied by Cristea and Steinsky [8, 9, 10, 12, 13] and some of the results were extended in recent research [14, 15] to even more general fractal objects called mixed labyrinth fractals. Studying these objects is of interest not just for mathematics, but also for research in physics, where some of the results have already been used, e.g., [36, 22, 37].

In this paper we present results on topological and geometrical properties that were obtained for the three families of Sierpiński carpets mentioned above, such as connectedness or lengths of arcs in these fractals, everything being done under a combinatorial frame, where the combinatorial character of the problems comes from the combinatorics of the generator(s) of the carpet: the pattern(s).

Although originally net sets and limit net sets were defined and constructed by means of net matrices [8], and the labyrinth fractals by using labyrinth sets [12, 13], throughout this paper we give a unifying approach of all the families of carpets mentioned above by means of patterns, as it was done in the case of the generalised Sierpiński carpets that were studied [9, 10] after the other mentioned carpets, and in more recent work, for mixed labyrinth fractals [14, 15].

Graph directed constructions, see, e.g., [29], GDMS (Graph Directed Markov Systems, see, e.g., [30]), and random fractals [17, 28] also offer frameworks for studying the objects that occur along this paper. Finally, we mention that there are recent results and ongoing research on V-variable fractals, see e.g. [21], and several of the fractals studied and mentioned in this section can be approached within the frame of V-variable fractals. For V-variable fractals and super-fractals we also refer to Barnsley's book [4].

Let us now give a short outline of the paper. In Section 1.2 we define planar patterns and the graph associated to a planar pattern. Section 1.3 is dedicated to net sets and limit net sets. In Section 1.4 we briefly present recent research on generalised Sierpiński carpets. Section 1.5 deals with results about self-similar and mixed labyrinth fractals and also refers to very recent results. Finally, Section 1.6 is dedicated to conclusions and final remarks of the survey.

1.2 Planar patterns and Sierpiński carpets

First, let us recall the definition of a pattern, as it is given in some of the above mentioned papers [9, 10]. Let $x, y, q \in [0,1]$ such that $Q = [x, x+q] \times [y, y+q] \subseteq [0,1] \times [0,1]$. Then for any point $(z_x, z_y) \in [0,1] \times [0,1]$ we define the function $P_Q(z_x, z_y) = (qz_x + x, qz_y + y)$.

Let $m \geq 1$. For the integers i, j with $0 \leq i, j \leq m-1$, let $S_{i,j}^m = \{(x,y) \mid \frac{i}{m} \leq x \leq \frac{i+1}{m}$ and $\frac{j}{m} \leq y \leq \frac{j+1}{m}\}$, and $\mathcal{S}_m = \{S_{i,j}^m \mid 0 \leq i \leq m-1$ and $0 \leq j \leq m-1\}$. We call any nonempty $\mathcal{A} \subseteq \mathcal{S}_m$ an $m \times m$ *pattern* or, in short, *m-pattern*.

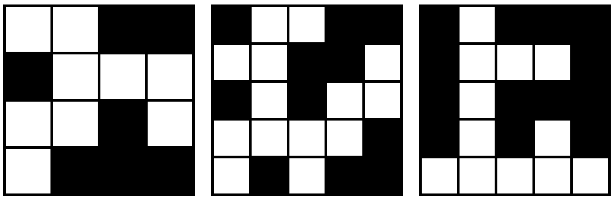

Figure 1: Three patterns, $\mathcal{A}_1$ (a 4-pattern), $\mathcal{A}_2$ (a 5-pattern) and $\mathcal{A}_3$ (a 5-pattern)

In Figure 1 we show three such patterns that are in particular also labyrinth patterns, which we define in Section 1.5. We mention that throughout this paper we think of the black regions in the figures as being "cut out" at the corresponding step, and subsequently the closure (with respect to the topology induced by the Euclidean metric in the plane) of the remainder set is taken.

All families of fractals that we present in this paper can be constructed by means of patterns, and in each case we use an iterative construction, analogous to that described in Section 1.1 for a Sierpiński carpet.

For any pattern $\mathcal{A} \subseteq \mathcal{S}_m$, we define the graph $\mathcal{G}(\mathcal{A}) \equiv (\mathcal{V}(\mathcal{G}(\mathcal{A})), \mathcal{E}(\mathcal{G}(\mathcal{A})))$ to be *the graph of* $\mathcal{A}$, i.e., the graph whose vertices are the (closed) white squares in $\mathcal{A}$, i.e., $\mathcal{V}(\mathcal{G}(\mathcal{A})) = \mathcal{A}$ and whose set of edges $\mathcal{E}(\mathcal{G}(\mathcal{A}))$ consists of the unordered pairs of white squares, that share a common side.

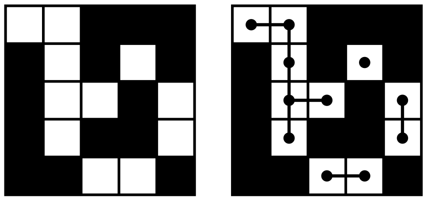

Figure 2: A 5-pattern $\mathcal{A}$ on the left, and the pattern with its corresponding graph $\mathcal{G}(\mathcal{A})$ on the right

1.3 Limit net sets

Net set and *limit net set* are new concepts developed in [8], based, on the one hand, on the observation that various porous materials present holes that at each scale are "evenly" distributed, and, on the other hand, on the distribution properties of (t, m, s)-nets, that are well distributed point sets in the unit cube, for more details see [33].

Originally, the net sets were defined [8] with the help of *net matrices*, that are 4×4 matrices having all entries from the set $\{0, 1\}$. Here we give a (shorter) equivalent definition of the net sets, that is appropriate for the framework of the present paper. We call a 4×4 pattern a *net pattern* if each of the four columns and each of the four rows (each containing four squares) contains exactly one black square, and inside each of the four subsquares of side-length $\frac{1}{2}$ of the unit square that share one vertex with the unit square there lies exactly one of the black squares mentioned above. There exist 16 such net patterns, four of them are shown in Figure 3, the other 12 can be obtained by flipping or rotating these. The union of all (closed) white squares in a given net pattern is the corresponding net set of level 0.

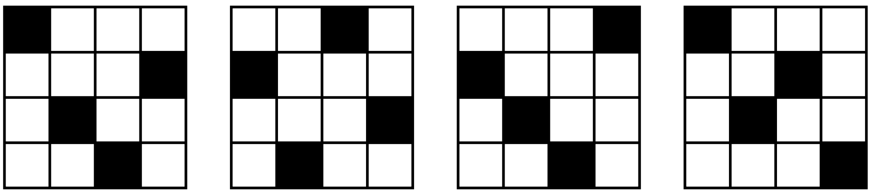

Figure 3: Examples of net patterns

The iterative construction of a sequence of nested sets (*net sets of level* $1, 2, \ldots$) is analogous to that described in the introduction of Section 1.1 for the Sierpiński carpets, but there is one essential difference: each white square of some level can be replaced, by a so-called *net substitution*, by any net set of level 0 scaled correspondingly, such that different white squares can be replaced by different net sets.

We call a net substitution *uniform* if all white squares of a net set of some level are substituted by the same scaled net set. Correspondingly, a net set of some level $k \geq 1$ is uniform if at each step of its construction a uniform net substitution (not necessarily the same) was applied.

Thus, by starting with a net pattern and the corresponding net set E_0 of level 0, one obtains, by applying net substitutions, a decreasing sequence of net sets $E_0 \supset E_1 \supset \ldots E_{k-1} \supset E_k \supset \ldots$.

The fractal $E_\infty := \bigcap_{k\geq 0} E_k$ obtained as the limit set of this construction is called the *limit net set* of the sequence $\{E_k\}_{k\geq 0}$ and can be viewed as the limit set of a Moran construction [32, 35, 28] with Hausdorff and box-counting dimension $1 + \frac{\log 3}{\log 4}$.

If at each step of the construction we apply a uniform net substitution, not necessarily the same, then the sets E_k of the above sequence are called *uniform net sets*, and E_∞ is called a *uniform limit net set*. A *totally uniform net set* is obtained if all substitutions use the same pattern, i.e., we apply the same net substitution at all steps, for all white squares. In this case the obtained limit net set is self-similar: it is a Sierpiński carpet (as defined in the introduction).

When studying connectedness properties of net sets and limit net sets, it is essential to identify two types of patterns: connected and disconnected net patterns. In terms of the graph of the pattern a connected net pattern is a pattern whose graph is connected. Otherwise, the net pattern is called disconnected.

Among other, it was proven that connected net patterns (or, originally, connected net matrices [8]) always produce connected limit net sets. For example, in Figure 3, the first, second and fourth net pattern are connected, while the third is a disconnected net pattern.

Criteria for different "degrees" of connectedness of these fractals have been proven. There are four different possible connectedness "degrees" for limit net sets: net-connectedness (a notion introduced in [8]), connectedness, disconnectedness and total disconnectedness [8]. It was shown how the connectedness or disconnectedness of the net patterns involved in the iterative construction affects the connectedness "degree" of the resulting fractal. Necessary and sufficient conditions for the net-connectedness of the fractal were proven, as well as necessary and sufficient conditions for the total disconnectedness of the fractals, necessary and sufficient conditions for a uniform limit net set to be connected, but not totally disconnected, or connected (in the Euclidean sense), but not net-connected.

Moreover, an analogon of fractal percolation in the unit cube (see, e.g., [27, 18, 17]), called *net percolation*, has been introduced, and a sufficient condition for net percolation was proven [8].

The results obtained for limit net sets provide methods for the construction of random fractals with a certain type of "well distributed" structure (holes) by using net patterns/net matrices, but also for constructing percolating fractal sets and sets that have certain connectedness properties.

Later on this idea of identifying families of patterns according to their shape was used [10] in the study of the generalised Sierpiński carpets to which the next section is dedicated.

1.4 Generalised Sierpiński carpets

Generalized Sierpiński carpets are planar sets in the unit square that were introduced and studied in [9, 10]. These sets generalise the Sierpiński carpets mentioned in the introduction. They differ in several aspects from a Sierpiński carpet defined as above: on the one hand, instead of using a single generating pattern, here we use a sequence of patterns in order to construct the generalised carpet, on the other hand, at any step k of the construction, a $m_k \times m_k$ pattern is used, where $m_k \geq 2$, for all $k \geq 1$, and, moreover, at any two steps $k_1 \neq k_2$ we may have distinct patterns, with $m_{k_1} \neq m_{k_2}$. Thus, generalised Sierpiński carpets are in general not self-similar. With the notations from Section 1.2 we introduce the following notions.

Let $\{\mathcal{A}_k\}_{k=1}^{\infty}$ be a sequence of non-empty patterns and $\{m_k\}_{k=1}^{\infty}$ be the corresponding *width-sequence*, i.e., for all $k \geq 1$ we have $\mathcal{A}_k \subseteq \mathcal{S}_{m_k}$. We let $\mathcal{W}_1 = \mathcal{A}_1$, and call it the *set of white squares of level* 1. For $n \geq 2$ we define the *set of white squares of level* n by

$$\mathcal{W}_n = \bigcup_{W \in \mathcal{A}_n, W_{n-1} \in \mathcal{W}_{n-1}} \{P_{W_{n-1}}(W)\}.$$

By defining three types of graphs associated to the patterns that generate the generalised Sierpiński carpets, necessary and sufficient conditions for the connectedness (with respect to the usual topology of the Euclidean plane) of these objects were proven [9].

A different approach, namely identifying certain *families of patterns*, was used [10] in order to study the structure of the sets obtained at the nth iteration in the construction of a generalised carpet, for $n \geq 1$, and it was shown that certain families of patterns provide total disconnectedness of the resulting fractals. Moreover, analogous results hold even in a more general setting [10]. This approach of the carpets provides the possibility

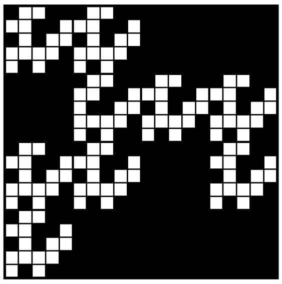

Figure 4: The set $\mathcal{W}_2$, constructed based on the patterns $\mathcal{A}_1$ and $\mathcal{A}_2$ shown in Figure 1, that can also be viewed as a 20-pattern

to construct disconnected carpets of box-counting dimension less than or even equal to 2, as it is shown in an example in the more extended arXiv-version [11] of the published paper [10].

The results on connected generalised carpets [9] and on distances between points on the "classical" s-dimensional carpet [7] were extended in more recent work by Hoffmann [23]: analogues of the generalised Sierpiński carpets mentioned above, called *generalised Sierpiński hypercubes*, were defined and studied, and it has been shown that these sets are uniformly regular, i.e., the geodesic metric is comparable to the Euclidean metric. We also mention that in previous work, several authors [2, 6, 24, 31, 34] studied objects called *general Sierpiński carpets* with respect to dimension and Hausdorff measure using rectangles instead of squares in the definition. While some of these carpets are self-affine, those defined by Barański [2] are not self-affine.

More recently, geometrical and topological properties of *fractal squares*, which are self-similar Sierpiński carpets as defined in the introduction, were studied [25, 39]. We note that the self-similar version of the limit net sets mentioned in Section 1.3 and the labyrinth fractals mentioned in Section 1.5 are fractal squares. Lau, Luo, and Rao [25] study the topological structure of a fractal square by studying the connected components. Moreover, recently there is considerable interest to study the Lipschitz equivalence of Cantor sets and of totally disconnected fractal squares, e.g., [26, 38].

In more recent work [14] dedicated to mixed labyrinth fractals, Steinsky and Cristea gave an other sufficient condition for the total disconnectedness of certain classes of generalised Sierpiński carpets, that occur in relation labyrinth fractals that we present in Section 1.5.

We note the combinatorics-flavoured approach of carpets by identifying special families among the generating patterns that provide certain properties, which was inspired by the results that were obtained for limit net sets, that is different from the approaches of other authors who have studied similar objects. On the other hand, Cristea and Steinsky used graphs a lot as a tool in order to characterise some properties of the patterns or of the prefractals obtained at some (finite) steps of the iterative construction of generalised Sierpiński carpets [9] or other carpets [12, 13, 14], and graphs were also used by other authors, e.g., when dealing with fractal squares [25].

1.5 Labyrinth fractals

An other new family of (self-similar) fractals, called *labyrinth fractals*, were introduced and studied during the last decade [12, 13]. These fractal objects are (self-similar) dendrites and a special case of the Sierpiński carpets mentioned at the beginning of Section 1.1. First, self similar labyrinth fractals generated by a 4×4 labyrinth pattern were studied [12]. Originally, such a generator was called "labyrinth set" [12], not "labyrinth pattern", as used in later work on mixed labyrinth fractals [14, 15]. Subsequently, by proving several quite technical lemmas and theorems, the results were extended [13] to the case of self-similar labyrinth fractals generated by $m \times m$ labyrinth patterns, for any $m \geq 5$.

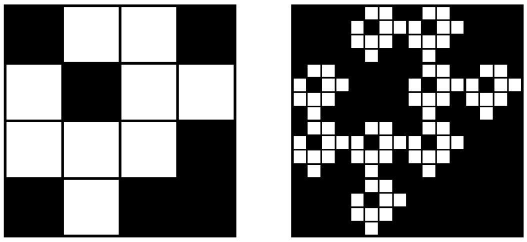

Figure 5: A 4×4 labyrinth pattern and the corresponding labyrinth set of level 2 (that can also be viewed as a 16×16 labyrinth pattern)

To the $m \times m$ pattern that generates a labyrinth fractal we associate the set of $\mathcal{W}_1$ of its (closed) white squares and call it the *set of white squares of level 1* or labyrinth set of level 1, and we define $L_1 = \cup_{W \in \mathcal{W}_1}$. By the iterative construction described in Section 1.1 we then obtain the sequence $\{\mathcal{W}_n\}_{n \geq 1}$, with $\mathcal{W}_n \subset \mathcal{S}_{m^n}$, and the decreasing sequence of compact sets $\{L_n\}_{n \geq 1}$.

A *top exit* in $\mathcal{W}_n$ is a white square in the top row of $\mathcal{W}_n$, such that there is also a white square in the same column in the bottom row. The *bottom exit*, *left exit*, and *right exit* are defined analogously.

A non-empty m-pattern $\mathcal{A} \subseteq \mathcal{S}_m$, $m \geq 3$ is called a $m \times m$*-labyrinth pattern* (in short, *labyrinth pattern*) if $\mathcal{A}$ satisfies satisfies the following three properties:

(1) $\mathcal{G}(\mathcal{W}_n)$ is a tree;

(2) exactly one top exit in $\mathcal{W}_n$ lies in the top row (of order n), exactly one bottom exit lies in the bottom row, exactly one left exit lies in the left column, and exactly one right exit lies in the right column;

(3) if there is a white square in $\mathcal{W}_n$ at a corner of $\mathcal{W}_n$, then there is no white square in $\mathcal{W}_n$ at the diagonally opposite corner of $\mathcal{W}_n$.

We note that the graph $\mathcal{G}(\mathcal{A})$ introduced in Section 1.2 can also be defined in the case $\mathcal{A} = \mathcal{W}_n$, $n \geq 1$. These graphs play an important role throughout the study of labyrinth sets and labyrinth fractals.

For any labyrinth pattern $\mathcal{A}$ and any integer $n \geq 1$, the *labyrinth set* (of level n) $\mathcal{W}_n$ has the above properties (1) - (3) of a labyrinth pattern [12].

The limit set L_∞ of the decreasing sequence of compact sets $\{L_n\}_{n\geq 1}$ is called a *labyrinth fractal*. Every labyrinth fractal has four exits. The top exit of L_∞ lies on the top edge of the unit square and is the intersection (point) $\cap_{n=1}^{\infty} T_n$, where T_n is the top exit in $\mathcal{W}_n$, for all $n \geq 1$. The bottom exit, the left and the right exit of L_∞ are defined analogously and lie correspondingly on the other edges of the unit square.

We say that an $m \times m$-labyrinth pattern $\mathcal{A}$ is *horizontally blocked* if the row (of squares) from the left to the right exit of $\mathcal{A}$ contains at least one black square, and it is called *vertically blocked* if the column (of squares) from the top to the bottom exit contains at least one black square. We remark that in Figure 1 the first two labyrinth patterns are both horizontally and vertically blocked, and the third pattern is neither horizontally, nor vertically blocked, while the 4×4 pattern shown in Figure 5 is both vertically and horizontally blocked. For more examples we refer to [12, 13, 14, 15].

Both topological and geometrical properties and aspects of the labyrinth sets and fractals were studied. It was proven that any self-similar labyrinth fractal L_∞ is a dendrite, i.e., a locally connected continuum that contains no simple closed curve [12, 13].

Subsequently, the arcs in L_∞ that connect exits of the fractal were studied, with emphasis on their length. In order to obtain results for the lengths of such arcs, we studied the lengths of paths in the tree $\mathcal{G}(\mathcal{W}_n)$ between exits in $\mathcal{W}_n$. Therefore, the *path matrix* M of the labyrinth set $\mathcal{W}_1$ was introduced, which is a 6×6 matrix where each entry represents the number of a certain type of squares in one of the 6 paths in $\mathcal{G}(\mathcal{W}_1)$ between two exits of $\mathcal{W}_1$. (For more details on the possible 6 types of squares in a path in $\mathcal{G}(\mathcal{W}_1)$ see, e.g., [12].) The path matrix plays an essential role and is a powerful instrument when dealing with lengths of paths in $\mathcal{G}(\mathcal{W}_n)$ and with lengths of arcs between exits in L_∞. Moreover, this matrix actually is the matrix of a substitution.

In order to prove the obtained results, several known theorems from different areas of mathematics were used: the Perron-Frobenius Theorem, the Hahn-Mazurkiewicz-Sierpiński Theorem (that characterises local connectedness), the Jordan Curve Theorem, and a labyrinth version of the Steinhaus Chessboard Theorem, proven in [12].

It was essential to establish [12, 13] a recursion and prove that the n-th power M^n of the path matrix gives information about the lengths of paths in $\mathcal{G}(\mathcal{W}_n)$. Moreover, it was shown that the path matrix of a $m \times m$- labyrinth pattern (or set) is primitive if and only if the pattern (set) is horizontally and vertically blocked. Then, the Perron-Frobenius Theorem for primitive matrices was used, see e.g. [40, Theorem 1.1, p.3], in order to obtain the asymptotics of the path lengths in $\mathcal{G}(\mathcal{W}_n)$ as n tends to infinity. This subsequently lead to results about the lengths of arcs in the labyrinth fractals generated by both horizontally and vertically blocked labyrinth patterns. In the case of $m \times m$-patterns with $m \geq 5$, not just the path matrix mentioned above, but also use a second matrix, the reduced path matrix, was used in order to prove the infinite length of arcs in the fractal [13].

The main results on labyrinth fractals, both in the case when the fractal is generated by a 4×4 pattern and in the case when the generating pattern is $m \times m$, with $m \geq 5$, are contained in the following theorem [12, 13].

Theorem. *If L_∞ is the labyrinth fractal generated by a horizontally and vertically blocked $m \times m$-labyrinth pattern ($m \geq 4$) with path matrix M, and r is the spectral radius of M, then between any two points in L_∞ there is a unique arc $\boldsymbol{a}$, the length of $\boldsymbol{a}$ is infinite, and the set of all points, at which no tangent to $\boldsymbol{a}$ exists, is dense in $\boldsymbol{a}$. Moreover, if $\boldsymbol{a}$ is an arc between two distinct points in L_∞ then its box-counting dimension is $\dim_B(\boldsymbol{a}) = \frac{\log(r)}{\log(m)}$.*

The case when the labyrinth fractal is generated by a 4×4-pattern that is blocked only in one direction (e.g., only horizontally, but not vertically blocked) is also interesting: we have proven that then there exist both arcs of finite length and arcs of infinite length in the fractal. Moreover, in this case the box-counting dimension of every arc is 1, while in the case of a labyrinth fractal generated by a both horizontally and vertically blocked pattern the dimension of such arcs is always strictly greater than 1. For more details we refer to [12].

Mixed labyrinth fractals were defined and studied later [14], as a generalisation of the self-similar labyrinth fractals mentioned above. Here, the construction is analogous to that of the generalised Sierpiński carpets mentioned in Section 1.4, with the difference that all patterns that occur throughout the construction are labyrinth patterns. In other words, mixed labyrinth fractals are a special case of generalised Sierpiński carpets. As an example, Figure 4 shows the labyrinth set of level 2, $\mathcal{W}_2$, generated by the patterns $\mathcal{A}_1$ and $\mathcal{A}_2$ from Figure 1.

Mixed labyrinth fractals are, like the self-similar labyrinth fractals mentioned above, dendrites [14], but here things get more complicated when studying lengths of paths in the graphs of mixed labyrinth sets of some level, and a lot more complicated when studying lengths of arcs in the fractal. The methods used in the self-similar case, based on the path matrix, can only be applied up to a certain point in the reasoning. This is due to the fact that in the self similar case the path matrix of a labyrinth set of level n is just M^n, where M is the path matrix of the generating pattern, while in the mixed case it is $M_1 \cdot M_2 \cdot M_n$, where M_k is the path matrix of the pattern $\mathcal{A}_k$, for $k = 1, \ldots, n$. Since there are no restrictions regarding the labyrinth patterns that occur in the generating sequence $\{\mathcal{A}_k\}_{k\geq 1}$, the methods used in the self-similar case in order to establish results on the asymptotical behavior of the path matrix associated to the labyrinth set of level n, for $n \to \infty$, cannot be applied here anymore, as soon as the sequence contains more than one pattern (unless the sequence is periodic, which is in general not the case). Moreover, there are also other properties that get lost when we give up self-similarity, e.g., in the case of mixed labyrinth fractals it is possible that an exit of the fractal lies, for some $n \geq 1$, in more than one white square of level n of $\mathcal{W}_n$, while in the self-similar case each exit lies in a unique such white square of level n.

In a recently published paper [15] in was shown, that in the case of a mixed labyrinth fractal the theorem stated above does not hold. More precisely, one can prove the following two results.

Theorem. *There exist sequences $\{\mathcal{A}_k\}_{k=1}^{\infty}$ of (both horizontally and vertically) blocked labyrinth patterns, such that the limit set L_∞ has the property that for any two points in L_∞ the length of the arc $a \subset L_\infty$ that connects them is finite. For almost all points $x_0 \in a$ (with respect to the length) there exists the tangent at x_0 to the arc a.*

Proposition. *There exist sequences $\{\mathcal{A}_k\}_{k=1}^{\infty}$ of (both horizontally and vertically) blocked labyrinth patterns, such that the limit set L_∞ has the property that for any two points in L_∞ the length of the arc $a \subset L_\infty$ that connects them is infinite.*

These results were proven by using a special family of labyrinth patterns, which we called "special cross patterns". An example of such a pattern is shown in Figure 6.

Here, the idea was to approximate the arcs that connect exits in the labyrinth fractal by special curves, which are related to the patterns used in the construction. For more details we refer to the paper [15]. Analogously to the self-similar case, by chosing suitable labyrinth patterns that are blocked in only one direction (e.g., horizontally but not vertically blocked), one can construct also in the mixed case labyrinth fractals where both arcs of finite length and arcs of infinite length exist between their points.

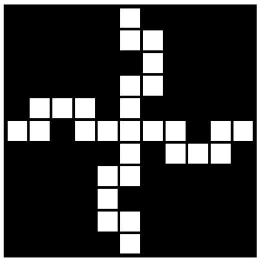

Figure 6: An example: a special cross pattern with width 11

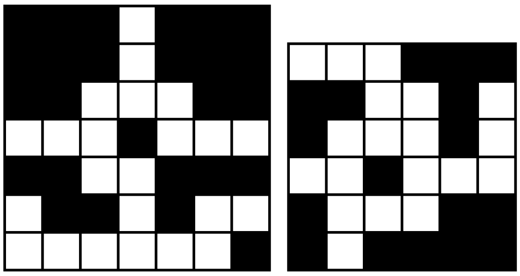

Figure 7: Examples: two wild labyrinth patterns, both vertically and horizontally blocked

The following conjecture was formulated [15]:
Conjecture. *A sequence of both horizontally and vertically blocked labyrinth patterns with the property that the sequence of widths* $\{m_k\}_{k\geq 1}$ *is bounded, generates a mixed labyrinth fractal with the property that for any* $x, y \in L_\infty$ *the length of the arc in the fractal that connects* x *and* y *is infinite.*

Finally, let us mention that in [14] it is also shown how, by relaxing the conditions imposed on the labyrinth patterns in order to construct *wild labyrinth patterns* and, correspondingly, (self-similar or mixed) *wild labyrinth fractals*, several properties of the labyrinth sets and fractals change, and in general the path matrices can not be used anymore in order to provide reliable information and results about the paths in the graphs of the labyrinth sets $\mathcal{G}(\mathcal{W}_n)$, for $n \geq 2$ or the lengths of arcs in the fractal. Figure 7 shows two wild labyrinth patterns. The first one has more than one horizontal exit pair, and the graph of the second one is only connected, but not a tree. Moreover, the connected net patterns mentioned in Section 1.3 are in particular 4×4 wild labyrinth patterns.

1.6 Conclusions

Although the fractals presented in this paper, limit net sets, generalised Sierpiński carpets and labyrinth fractals, can also be studied by using other approaches than the one used here, e.g., under the framework of IFS, graph-directed constructions, GDMS, random fractals or V-variable fractals, here we chose this unifying and rather combinatorial approach based on planar patterns. The motivation of this fact is that, in our opinion, this is a way to bring them closer to other sciences, to specialists from other fields, to a wider audience in general, since the notion of "pattern" is very intuitive, wide-spread (even in every day life) and somehow basic for the understanding. Moreover, as it follows from the cited papers, patterns are sufficient in order to construct and study these new, special families of fractals with remarkable properties.

The idea is that in this approach mainly by identifying families of patterns or a few properties of the patterns that are easy to check, one can generate fractals of prefractals with desired topological or geometrical properties (like types or degrees of connectedness, or lengths of arcs between points in the fractal), or, in addition, with desired fractal dimension.

It is important to add here that physicists use fractals like those mentioned above as models in different areas, e.g, for the study of materials or of diffusion in porous matter [20, 42, 36], planar nanostructures [22], or even for the construction of new, more performant devices (e.g. radar antennas) [37].

In this context it is worth to remark that, while the mathematicians focus mainly on the fractal, i.e., on the objects obtained as the limit of the iterative construction, the physicists are usually more interested in some prefractal obtained after a high enough number of iterations. In other words, while the mathematicians are mainly interested in what happens in the infinite, in the limit, the physicists are interested in what is obtained at a finite step that approximates the limit well enough, or where the scale is fine enough, but not infinitely fine. Let us give an example. From the point of view of research in physics, the properties (1) and (2) of labyrinth patterns are essential, and they are sufficient, since the property (3) of labyrinth patterns only plays a role in the limit, when dealing with the resulting labyrinth fractal: the fact that the resulting labyrinth fractal is a dendrite played an essential role when proving some of the other results, e.g., those on the length of arcs in the fractal.

Finally, let us mention that due to the interesting properties of limit net sets, generalised Sierpiński carpets and labyrinth fractals, at the moment this research is continued on new families of fractals, that are further generalisations of the objects mentioned here: there is a lot of magic and still a lot to discover in this field.

1.7 Acknowledgment

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Secondary structures and some related combinatorial objects

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Abstract

A secondary structure is a (planar, labeled) graph on the vertex set $[n]$ having two kind of edges: the segments $[i, i+1]$, for $1 \leq i \leq n-1$, and arcs in the upper half-plane connecting some vertices i, j, where $j - i > l$, for some fixed integer l. Any two arcs must be totally disjoint. We establish connections between secondary structures and some well known combinatorial families, such as lattice paths, matchings and restricted permutations. Then we give some applications and connections with polygon dissections and polyominoes, using earlier enumerative results on secondary structures to provide explicit formulas and asymptotics for enumerating sequences of those families.

Keywords: secondary structure; Motzkin path; Dyck path; polygon dissection; restricted permutation

MSC: 05A15; 05A16; 05A20; 05B50; 05C30; 05C70; 33C45; 92D20

1.1 Introduction

Many interesting and important molecules belong to the class of linear polymers. That means they are long chains built from simpler building blocks called monomers. For example, proteins are chains of amino-acids. DNA molecules are linear polymers too, as well as closely related molecules of RNA. They together make the class of nucleic

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acids, and their building blocks are called **nucleotides**. The nucleic acids are essential for coding, transferring and retrieving genetic information, and also in directing cell metabolism. In this paper we will look at RNA molecules.

RNA molecules are single-stranded and their nucleotides belong to one of four types. Those four type of nucleotides differ by only one part, called **base**. There are four different types of bases, denoted by letters A, C, G, and U. As we are not interested in details of their structure, we usually identify nucleotides with bases and use the same four letters for denoting nucleotides.

Nucleotides are polar molecules with two differing ends, usually denoted by 5' and 3'. The 5' end of one nucleotide readily binds to the 3' end of another nucleotide by a phosphorus bond (or a p-bond). In that way, nucleotides form chains in which each of them (except the two terminal ones) is connected to exactly two neighbors via p-bonds. Those p-bonds form the **backbone** of the molecule. The sequence of nucleotides (or bases), read from the terminal nucleotide with free 5' end, is the **primary structure** of the molecule. The total number of all possible primary structures of a molecule with n nucleotides is equal to 4^n.

However, certain pairs of bases, such as C and G, A and U, and G and U, have an affinity to each other that enables them to bind via hydrogen bonds or h-bonds. Those bonds, when formed, cause folding of the molecular backbone into three-dimensional configurations that minimize potential energy. Some of the folded configurations remain planar; they are called **secondary structures** of an RNA molecule. Non-planar foldings are called **tertiary structures**. Both secondary and tertiary structures contribute to the shape of a folded molecule and thus determine its biological function. In this paper we look only at secondary structures.

The secondary structures of a given molecule are subject to certain stereo-chemical constraints. First, no base can participate in more than one h-bond. Second, a base cannot be paired by an h-bond to a base that is too close along the backbone, due to the rigidity of the backbone's p-bonds. Third, and the most important, constraint on h-bonds is that they may not cross. It means that, if there is an h-bond pairing the bases i and j, and an h-bond pairing the bases k and l, then either $i < j < k < l$ or $i < k < l < j$. In biological terminology, this constraint prohibits **pseudo-knots**.

Besides their importance in molecular biology, secondary structures are also interesting from the mathematical point of view. We refer the reader to several papers dealing with various aspect of their mathematics [11, 15, 19, 20, 23, 24]. In particular, we will rely here on several structural and enumerative results established in [7, 8, 9].

The most suitable context for combinatorial modeling of secondary structures is the graph theory. We represent the bases by vertices, and the bonds by edges of certain graphs. The stereo-chemical constraints translate quite naturally into the graph-theoretical language. We refer the reader to [25] for all graph-theoretical terms not defined here.

Let n and l are integers, $n \geq 1$, $l \geq 0$. A **secondary structure** of **size** n and **rank** l is a labeled non-oriented graph S on the vertex set $V(S) = [n] = \{1, 2, ..., n\}$ whose edge set $E(S)$ consists of two disjoint subsets, $P(S)$ and $H(S)$, satisfying the following conditions:
(a) $\{i, i+1\} \in P(S)$, for all $1 \leq i \leq n-1$;
(b) $\{i, j\} \in H(S)$ and $\{i, k\} \in H(S) \Longrightarrow j = k$;
(c) $\{i, j\} \in H(S) \Longrightarrow |i - j| > l$;
(d) $\{i, j\} \in H(s), \{k, l\} \in H(S)$ and $i < k < j \Longrightarrow i < l < j$.

Obviously, the set $P(S)$ contains the edges corresponding to the p-bonds of the molecule's backbone. The set $H(S)$, which may be empty, contains the edges representing the h-bonds. A secondary structure S with $H(S) = \emptyset$ is called **trivial**. The number of edges in $H(S)$ is the **order** of S, and the parameter l is the structure's rank. The only secondary structure of size 1 is the graph K_1.

An example of a secondary structure of size 12, rank 1 and order 3 is shown on Fig.1. Note that every h-bond "leaps" over at least 1 base.

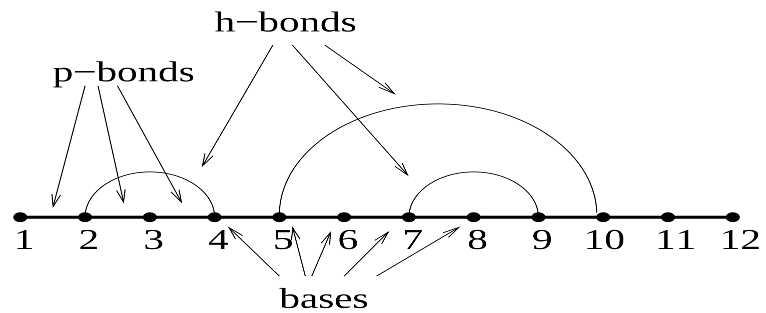

Figure 1: An example of a secondary structure

Some basic properties of secondary structures are stated in the following proposition.

Proposition 1 *[7] Let S be a secondary structure of size $n \geq 1$ and rank $l \geq 0$. Then*
(a) S is connected;

(b) S is simple for all $l \geq 1$;
(c) S is sub-cubic, i.e. $deg(v) \leq 3$ for all $v \in V(S)$;
(d) S is outerplanar;
(e) $girth(S) \geq l + 2$;
(f) the weak dual of S is a tree;
(g) $H(S)$ is a matching in S.

We denote the set of all secondary structures of size n and rank l by $\mathcal{S}^{(l)}(n)$, while the set of all such structures of order k is denoted by $\mathcal{S}_k^{(l)}(n)$. The cardinalities of these sets, i.e., their enumerating sequences, will be denoted by $S^{(l)}(n)$ and $S_k^{(l)}(n)$, respectively. By definition, $S^{(l)}(0) = 1$, for all l.

There are many ways of representing secondary structures graphically. Three of them, the loop diagram, the chord diagram and the arc diagram, are shown on Fig.2 a), b) and c), respectively.

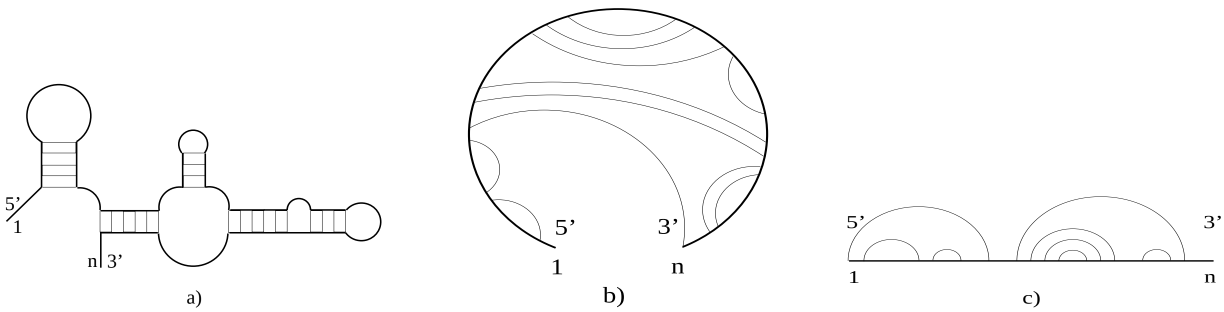

Figure 2: The loop diagram, the chord diagram and the arc diagram representations of secondary structures

1.2 Combinatorial context

In this Section we establish some connections between secondary structures and various well studied combinatorial families, such as lattice paths, matchings and permutations with forbidden patterns. We start with definitions of some important families of lattice paths and their enumerating sequences.

A **Dyck path** (or a "mountain path") of length $2n$ is a lattice path in the coordinate plane (x, y) from $(0, 0)$ to $(2n, 0)$ with steps $(1, 1)$ (Up) and $(1, -1)$ ($Down$), never falling below the x-axis. The number of steps in a Dyck path is called its **length** and it must be even. We denote the set of all Dyck paths of length $2n$ by $\mathcal{D}(n)$.

A **peak** of a Dyck path is a place where an *Up* step is immediately followed by a *Down* step. The set of all Dyck paths of length $2n$ with exactly k peaks ($1 \le k \le n$) is denoted by $\mathcal{D}_k(n)$.

It is well known that Dyck paths are enumerated by Catalan numbers, i.e. that $|\mathcal{D}(n)| = C_n$. (Recall that the n-th **Catalan number**, $C_n, n \ge 0$, is defined by $C_n = \frac{1}{n+1}\binom{2n}{n} = \frac{1}{2n+1}\binom{2n+1}{n}$. Hundreds of combinatorial families enumerated by Catalan numbers are listed in Exercise 6. 19 of [21] and in [22].)

A **Motzkin path** of length n is a lattice path in (x, y) plane from $(0, 0)$ to $(n, 0)$ with steps $(1, 1)$ (*Up*), $(1, -1)$ (*Down*) and $(1, 0)$ (*Level*), never falling below the x-axis. We denote the set of all Motzkin paths of length n (i.e. with exactly n steps) by $\mathcal{M}(n)$. The number $M_n = |\mathcal{M}(n)|$ is n-th **Motzkin number**. By definition, $M_0 = 1$. A typical member of the Motzkin family $\mathcal{M}(17)$ is shown on Fig.3.

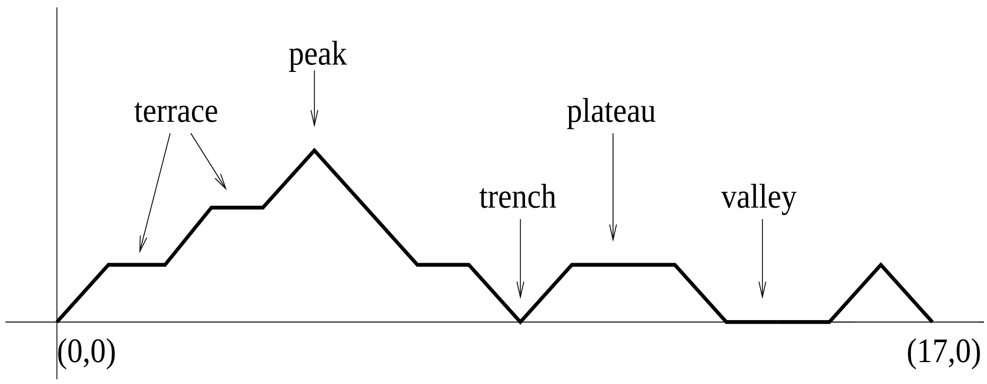

Figure 3: A Motzkin path of length 17

A **peak** of a Motzkin path is a place where an *Up* step is immediately followed by a *Down* step. A **plateau** of length l is a sequence of l consecutive *Level* steps, immediately preceded by an *Up* step, and immediately followed by a *Down* step. A sequence of $m \ge 0$ consecutive *Level* steps, immediately preceded by a *Down* step, and immediately followed by an *Up* step is called a **valley** of width m. If $m = 0$, we speak of a **trench**. A sequence of $m \ge 1$ consecutive *Level* steps, immediately preceded by a *Down* step, and directly followed by an *Up* step (or preceded by an *Up* step and followed by a *Down* step) is called a **terrace** of width m. In our example of Fig.3 we can see peaks at the points $(5, 3)$ and $(16, 1)$, a plateau of length 2 formed by the steps 11 and 12, terraces of width 1 formed by the steps 2, 4 and 8, a valley of width 2 formed by the steps 14 and 15, and a trench formed by the steps 9 and 10. We notice that a Dyck path is a Motzkin path without any *Level* steps.

Let us denote by $\mathcal{M}^{(l)}(n)$ the set of all paths from $\mathcal{M}(n)$ whose every plateau is at least l steps long. For $l = 0$ we get simply $\mathcal{M}^{(0)}(n) = \mathcal{M}(n)$. there is a bijective correspondence between $\mathcal{M}^{(l)}(n)$ and $\mathcal{S}^{(l)}(n)$.

Proposition 2 *There is a bijection between $\mathcal{M}^{(l)}(n)$ and $\mathcal{S}^{(l)}(n)$, for all $n \geq 1, l \geq 0$.*

This results belongs to mathematical folklore and was rediscovered several times. The proof is very simple. Indeed, take a secondary structure from $\mathcal{S}^{(l)}(n)$ and scan it from left to right. Assign a *Level* step to each unpaired base, an *Up* step to each base in which a new h-bond starts, and a *Down* step to each base in which an already encountered h-bond terminates. It is obvious that the lattice path obtained in this way never falls below the x-axis, that it has equally many *Up* and *Down* steps (and hence terminates at $(n, 0)$), and that at least l *Level* steps must be found between any *Up* and any *Down* step. So, this lattice path belongs to $\mathcal{M}^{(l)}(n)$. The injectivity of the construction is obvious.

The construction is easily seen to be invertible. Start from the first step in a path from $\mathcal{M}^{(l)}(n)$ and proceed toward the right constructing a secondary structure by assigning an unpaired base to each *Level* step. To an *Up* step assign a base in which an h-bond starts, and to a *Down* step assign a base in which the last-started h-bond terminates. Properties of Motzkin paths now ensure that so formed h-bonds will not cross and that the endpoints of any h-bond will be separated by at least l unpaired bases. So, we obtain a valid secondary structure in $\mathcal{S}^{(l)}(n)$, and the injectivity of the construction is, again, obvious.

It is clear from the above construction that the number of *Up* steps in the Motzkin path is equal to the order of the corresponding secondary structure. A secondary structure from $\mathcal{S}^{(1)}(12)$ and the corresponding Motzkin path from $\mathcal{M}^{(1)}(12)$ are shown in Fig.4.

It was shown in Proposition 1.2 of [8] that the correspondence can be extended also to some negative values of l. For example, there is a bijection between $\mathcal{S}^{(-1)}(n)$ and $\mathcal{D}(n + 1)$, where $\mathcal{S}^{(-1)}(n)$ is the set of all secondary structures on n bases in which an h-bond can form a loop, i.e., it may terminate in the same base it starts from. Of course, such mathematical objects do not correspond to biochemically realistic structures.

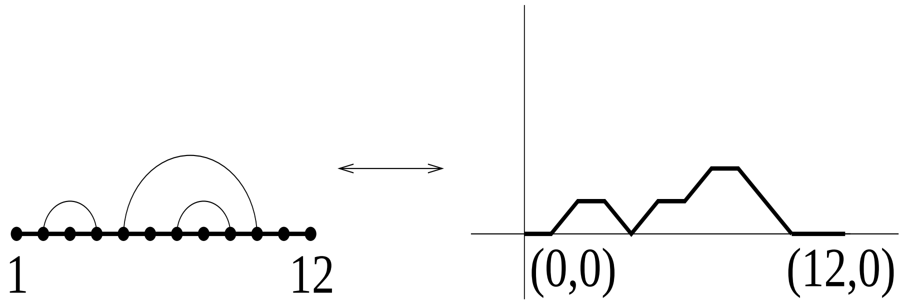

Figure 4: The folklore correspondence between secondary structures and Motzkin paths.

Let us now turn our attention to some other combinatorial interpretations of secondary structures. One of them reflects the fact that h-bonds form a matching in a secondary structure graph.

For a given graph G, a **matching** in G is any set M of edges of G such that no two edges from M have a vertex in common. From a given graph G we get its m-th power, G^m, by connecting by an edge any two vertices whose distance in G is at most m.

Now take a graph G and denote by G' one of its representations in the plane. A matching M is **non-intersecting** with respect to G' if edges from M do not intersect in G'. In Fig.5 we see two representations, G' and G'' of the same graph K_4, and a matching $M = \{ac, bd\}$ which is non-intersecting w.r.t G'', but not w.r.t G'.

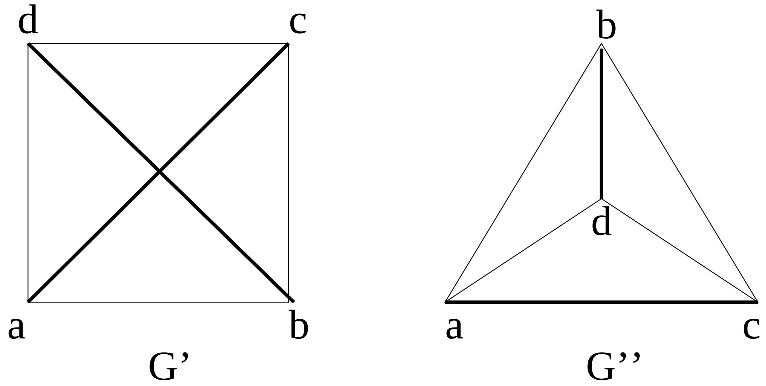

Figure 5: The same matching in two different representations of the same graph

Theorem 3 *There is a bijection between $\mathcal{S}^{(l)}(n)$ and the set of all matchings non-intersecting w.r.t. circular representation of $K_n - E(P_n^l)$, where P_n is a path on n vertices.*

Proof. Take a copy of K_n and represent it in the plane so that its vertices lie on a circle. Number them consecutively in, say, clockwise direction from 1 to n. Denote by P_n the path consisting of the edges of the form $\{i, i+1\}$, for $1 \leq i \leq n-1$, and remove all the edges of P_n^l. It is obvious that every remaining edge in this graph corresponds to a possible h-bond in a secondary structure in a molecule whose backbone corresponds to P_n. Any matching in this graph satisfies the conditions (b) and (c) in the definition of secondary structure, and non-intersecting matchings satisfy also the condition (d). So we can assign a secondary structure S of size n and $H(S) = M$ to every non-intersecting matching M in $K_n - E(P_n^l)$, and this assignment is obviously injective.

On the other hand, take a secondary structure S from $\mathcal{S}^{(l)}(n)$. From Proposition 1 we know that $H(S)$ is a matching, and by definition of secondary structure, this matching must be non-intersecting w.r.t circular representation of K_n. As no h-bond can connect bases whose distance is less than $l+1$, all permitted h-bonds must be edges in $K_n - E(P_n^l)$, where edges of P_n correspond to the molecule's backbone. ■

We conclude this section by pointing to a connection between secondary structures and pattern avoidance in permutations. A **pattern** is a permutation $\sigma \in \Sigma_k$, and a permutation $\pi \in \Sigma_n$ **avoids** σ if there is no subsequence in π whose members are in the same relative order as the members of σ. It is well known that the number of permutations from Σ_n avoiding $\sigma \in \Sigma_3$ is C_n, for all patterns $\sigma \in \Sigma_3$ [6].

The notion of pattern avoidance was generalized in [1], by allowing the requirement that two letters adjacent in a pattern must be adjacent in the permutation. An example of a generalized pattern is $1-32$, where an $1-32$ subword of a permutation $\pi = a_1 \dots a_n$ is any subword $a_i a_j a_{j+1}$ such that $i < j$ and $a_i < a_{j+1} < a_j$. Generalized pattern avoidance is treated in more detail in [4], where it is shown that the permutations from Σ_n that avoid both $1-23$ and $13-2$ are enumerated by the Motzkin numbers.

Proposition 4 *There is a bijection between $\mathcal{S}^{(l)}(n)$ and the set of all permutations from Σ_n that avoid*
$\{1-23, 13-2, ij\}$, where $j \leq i+l$, for all $l \geq 0$.

Proof. The claim follows by closer inspection of the bijection from the proof of Proposition 24 in [4]. It is easy to see that any pattern $i, i+k$ in a permutation $\sigma \in \Sigma_n$ avoiding

$\{1-23, 13-2\}$ generates a plateau of length $k-1$ in the corresponding Motzkin path.
■

1.3 Decomposable secondary structures

We now make a digression and consider a special class of secondary structures. A secondary structure is **decomposable** if there is a base whose removal leaves two valid secondary structures. (One, or even both of them may be empty.) In other words, a secondary structure is decomposable if there is a horizontal step on the x-axis in the corresponding Motzkin path. We would like to know how many of all secondary structures of given rank and size belong to the class of decomposable structures.

Denote by $\mathcal{D}^{(l)}(n)$, $\mathcal{U}^{(l)}(n)$ the sets of all decomposable and undecomposable secondary structures of rank l and size n, respectively. Put $D^{(l)}(n) = |\mathcal{D}^{(l)}(n)|$, $U^{(l)}(n) = |\mathcal{U}^{(l)}(n)|$.

Theorem 5 $U^{(l)}(n) = S^{(l)}(n) - U^{(l)}(n-1) - \ldots - U^{(l)}(n-l-1)$, *for* $n, l \geq 0$.

Proof. We first exhibit a bijection between $\mathcal{D}^{(l)}(n-1)$ and a certain subset $\mathcal{P}_n$ of $\mathcal{S}^{(l)}(n)$. The claim will then follow by analyzing the structure of $\mathcal{P}_n$. We describe the bijection in terms of Motzkin paths with plateaus of length at least l. Take a path Q from $\mathcal{D}^{(l)}(n-1)$ and consider its last (the rightmost) horizontal step on the x-axis. The sub-path on the right of this step we leave unchanged, and the rest we transform as follows. We replace the rightmost horizontal step by a *Down* step, we insert an *Up* step in front of the first (the leftmost) step, and we increase the altitudes of all intervening steps by one. In this way we obtain a path P from $\mathcal{U}^{(0)}(n)$. Put $P = \psi(Q)$. It is obvious that ψ is an injection. Denote by $\mathcal{P}_n$ the image of the set $\mathcal{D}^{(l)}(n-1)$ by the mapping ψ. Obviously, $|\mathcal{P}_n| = |\mathcal{D}^{(l)}(n-1)|$, and there is a function $\varphi : \mathcal{P}_n \to \mathcal{D}^{(l)}(n-1)$ such that $\varphi = \psi^{-1}$. The function φ acts as follows. For a given path $P \in \mathcal{P}_n$, consider its first return to the x-axis. Then transform the (elevated) sub-path on the left hand side of this return in the following way. Omit the first step (which was an *Up* step), replace the last step (a *Down* one) by a horizontal step on the x-axis, and translate all the steps in between one unit down. The sub-path of P on the right hand side of its first return to the x-axis leave unchanged. The path $\varphi(P)$ is obviously an element of $\mathcal{D}^{(l)}(n-1)$.
Now take a path from $\mathcal{U}^{(l)}(n)$. For any such path S we have $\varphi(S) \in \mathcal{D}^{(l)}(n-1)$, so $\mathcal{U}^{(l)}(n)$ must be a subset of $\mathcal{P}_n$. Are there any elements in $\mathcal{P}_n - \mathcal{U}^{(l)}(n)$? The answer is yes, because the function ψ can produce a path whose plateau length will be less than l.

But the only way to get such a path is to start from a path in $\mathcal{D}^{(l)}(n-1)$ beginning with a sequence of m consecutive horizontal steps on the x-axis, where $1 \leq m \leq l$. There are $U^{(l)}(n-1-m)$ such paths for any given m. So, the total of $\sum_{m=1}^{l} U^{(l)}(n-1-m)$ paths from $\mathcal{D}^{(l)}(n-1)$ will be mapped into elements of $\mathcal{P}_n - \mathcal{U}^{(l)}(n)$. Now we have

$$D^{(l)}(n-1) = U^{(l)}(n) + \sum_{m=1}^{l} U^{(l)}(n-1-m).$$

From $D^{(l)}(n-1) = S^{(l)}(n-1) - U^{(l)}(n-1)$ we get the claim. ■

Corollary 6 *There are equally many Motzkin paths of length n without horizontal steps on the x-axis and Motzkin paths of length $n-1$ with at least one horizontal step on the x-axis.*

This Corollary also gives a solution of Problem 10816 in [5], p.652.

1.4 Sequences $S^{(l)}(n)$ and $S_k^{(l)}(n)$

In this section we summarize the main results of reference [8]. In particular, we show how to obtain formulas for the number of secondary structures of given size, rank and order.

Some insight can be gained with little effort. It is clear that there is no secondary structure of order $k > \frac{n-l}{2}$, since each h-bond consumes 2 bases, and at least l bases must remain unpaired. Using the same arguments we can conclude that the structure of the maximal order is unique in a molecule whose size n has the same parity as the rank l. Also, for the molecules of size $n < l + 2$, only the trivial structure is possible. So, the numbers $S_k^{(l)}(n)$ will form a triangle in a table whose rows are indexed by n and columns by k. All non-zero elements of this table will be below the line $n - 2k = l$, except l 1's, counting the trivial secondary structures in molecules of size $n < l$.

Before we describe the solution of the problem of determining $S_k^{(l)}(n)$, some combinatorial preliminaries are in order.

First recall that Dyck paths are lattice paths from $(0, 0)$ to $(2n, 0)$ using only the steps $(1, 1)$ and $(1, -1)$, never falling below the x-axis. The set of all Dyck paths of length $2n$ we denote by $\mathcal{D}(n)$, and their number is C_n, the n-th Catalan number.

The **Narayana numbers** $N(n,k)$ are defined for integers $n,k \geq 1$ by

$$N(n,k) = \frac{1}{n}\binom{n}{k}\binom{n}{k-1} = \frac{1}{k}\binom{n}{k-1}\binom{n-1}{k-1},$$

with the initial value $N(0,0) := 1$ and the boundary values $N(n,0) = 0, N(n,1) = 1$ for $n \geq 1$.

It is well known that the Narayana numbers $N(n,k)$ enumerate Dyck paths of length $2n$ with exactly k peaks. This fact is instrumental in obtaining explicit formulas for $S_k^{(l)}(n)$.

Theorem 7 *[8]*

$$S_k^{(l)}(n) = \sum_{p=1}^{k} \frac{1}{k}\binom{k}{p}\binom{k}{p-1}\binom{n-lp}{2k}$$

$$S_k^{(l)}(n) = \sum_{p=1}^{k} N(k,p)\binom{n-lp}{2k}$$

for all $n, p, l \geq 0$.

Proof. Consider a Dyck path P on $2k$ steps with exactly p peaks. We know that there are $N(k,p)$ such paths. By inserting l horizontal steps between every two steps forming a peak, we get a path P' in $\mathcal{M}^{(l)}(2k+lp)$, the set of all Motzkin paths on $2k+lp$ steps with plateaus of length at least l. There are exactly $N(k,p)$ such paths. Now take additional m horizontal steps and distribute them at will in the path P'. From every path $P' \in \mathcal{M}^{(l)}(2k+lp)$ we can get $\binom{2k+m}{m}$ paths in $\mathcal{M}^{(l)}(2k+lp+m)$. Denoting the total number of steps by n, we get $N(k,p)\binom{n-lp}{2k}$ as the number of paths from $\mathcal{M}^{(l)}(n)$ which have exactly p plateaus. Summing over all p's from 1 to k, we get the number of paths in $\mathcal{M}^{(l)}(n)$ with k steps of the form $(1,1)$, whose all plateaus are at least l steps long. Recalling our correspondence between such Motzkin paths and secondary structures of rank l (Proposition 2), we get the claim of the theorem. ■

Corollary 8 $S_k^{(1)}(n) = N(n-k,k+1) = \frac{1}{k+1}\binom{n-k}{k}\binom{n-k-1}{k} = \frac{1}{n-k}\binom{n-k}{k}\binom{n-k}{k+1}$ *for all* $n,k \geq 0$.

The first few rows of the triangle of $S_k^{(1)}(n)$ numbers are given in Table 1. below. Closer look at this table reveals certain symmetry pattern. We see that $S_k^{(1)}(n) = S_{n-2k-1}^{(1)}(2n-3k-1)$. This symmetry is a consequence of the symmetry property of Narayana numbers. We give here a combinatorial proof of this property.

n \ k	0	1	2	3	4	5	6	$\Sigma = S_n$
0	1							1
1	1							1
2	1							1
3	1	1						2
4	1	3						4
5	1	6	1					8
6	1	10	6					17
7	1	15	20	1				37
8	1	21	50	10				82
9	1	28	105	50	1			185
10	1	36	196	175	15			423
11	1	45	336	490	105	1		978

Table 1: The beginning rows of the triangle $S_k^{(1)}(n)$

Proposition 9 *There is a bijection between the sets* $\mathcal{S}_k^{(1)}(n)$ *and* $\mathcal{S}_{n-2k-1}^{(1)}(2n-3k-1)$.

Proof. Take a secondary structure S from $\mathcal{S}_k^{(1)}(n)$. Map the structure S to a Dyck path P in $\mathcal{D}_{n-2k}(n-k)$. Now invoke the bijection $f : \mathcal{D}_{n-2k}(n-k) \to \mathcal{D}_{k+1}(n-k)$ that accounts for the symmetry property $N(n,k) = N(n, n+1-k)$ of Narayana numbers and map P into $P' \in \mathcal{D}_{k+1}(n-k)$. Finally, map the path P' back to a secondary structure. The obtained secondary structure lies in $\mathcal{S}_{n-2k-1}^{(1)}(2n-3k-1)$ and the correspondence is obviously bijective. ■

We say that the secondary structures from $\mathcal{S}_{n-2k-1}^{(1)}(2n-3k-1)$ are **dual** to the structures from $\mathcal{S}_k^{(1)}(n)$. The duality of sets $\mathcal{S}_1^{(1)}(5)$ and $\mathcal{S}_2^{(1)}(6)$ is illustrated on Fig. 6.

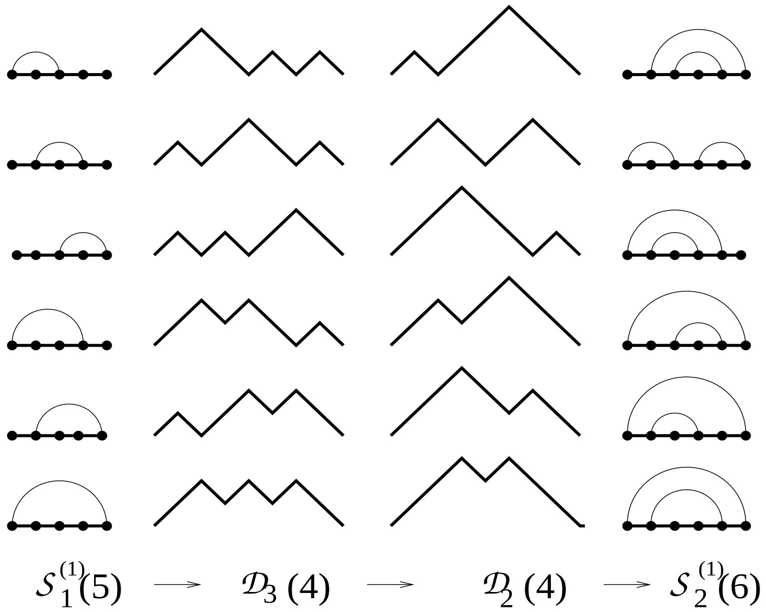

Figure 6: An example of dual sets of secondary structures

1.5 Some geometric applications

The various problems of polygon dissections have attracted much attention during last two centuries. Most of them require using of non-intersecting diagonals, i.e. diagonals which do not intersect in the interior of the considered polygon (e.g. [2, 3, 18]). Strengthening a little bit the condition of non-intersecting, and requiring that the the diagonals be totally disjoint, i.e. having no common point at all, we get an interesting variant of the polygon dissection problem, which, to the best of our knowledge, received no attention so far.

Problem

In how many ways one can dissect a convex n-gon using exactly k totally disjoint diagonals?

The problem also has an equivalent formulation as follows: How many ways are there of selecting k totally disjoint diagonals of an n-gon?

Let us denote the number of dissections of an n-gon by k totally disjoint diagonals by $D_k(n)$, and the total number of all such dissections of an n-gon by $D(n)$. Clearly,

$D(n) = \sum_{k=0}^{\lfloor \frac{n-2}{2} \rfloor} D_k(n)$. All the four dissections of an 8-gon by three totally disjoint diagonals are shown on Fig.7.

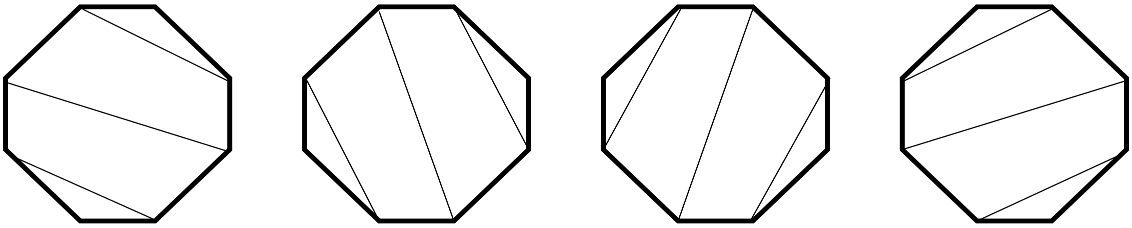

Figure 7: Dissections of an 8-gon with totally disjoint diagonals

We present here a simple solution of this problem, based on connections between the polygon dissections and secondary structures.

Theorem 10 $D_k(n) = \frac{n}{k(k+1)} \binom{n-k-2}{k} \binom{n-k-1}{k-1}$, *for all* $n \geq 3, 1 \leq k \leq \lfloor \frac{n-2}{2} \rfloor$.

Proof. Let us consider a secondary structure (of rank 1) of k-th order in a molecule with n bases, $k \geq 1$. If the considered structure contains an h-bond connecting the bases 1 and n, then the remaining $k-1$ h-bonds form a secondary structure in a molecule of size $n-2$. If the considered structure does not contain such an h-bond, then its h-bonds form a set of k totally disjoint diagonals in an n-gon obtained by adding the side $1-n$ to the molecule's backbone. From this observation we get $S_k^{(1)}(n) = S_{k-1}^{(1)}(n-2) + D_k(n)$, and then $D_k(n) = S_k^{(1)}(n) - S_{k-1}^{(1)}(n-2)$. The claim now follows by substituting the explicit value for $S_k^{(1)}(n)$ from Corollary 8. ■

Obviously, $D_0(n) = 1$, for all $n \geq 3$.

The numbers $D_k(n)$ form a triangular number array. We tabulate here its first few rows:

The following results are immediate consequences of Theorem 10:

Corollary 11

$$D(n) = S^{(1)}(n) - S^{(1)}(n-2), \qquad n \geq 3$$

$$\sum_{k \geq 0} D_k(n+k) = C_n - C_{n-1}, \qquad n \geq 3.$$

n k	0	1	2	3	4	5	6	$\Sigma = D_n$
1	0							1
2	1							1
3	1							1
4	1	2						3
5	1	5						6
6	1	9	3					13
7	1	14	14					29
8	1	20	40	4				65
9	1	27	90	30				148
10	1	35	175	125	5			341
11	1	44	308	385	55			793
12	1	54	504	980	315	6		1860
13	1	65	780	2184	1274	91		4395

Table 2: The beginning rows of the triangle $D_k^{(1)}(n)$

It can be checked by direct calculations that the numbers $D_k(n)$ are log-concave (and hence unimodal) in k. By expressing $D_k(n)$ in the form $D_k(n) = \frac{n(n-2k)(n-2k-1)}{(k+1)(n-k)^2(n-k-1)} \binom{n-k}{k}^2$, we can establish the following asymptotic behavior of the position of the maximal value of $D_k(n)$.

Proposition 12 *Let k_n be the value of k for which the maximal value of $D_k(n)$ is attained, for a fixed n. Then $\lim_{n\to\infty} \frac{k_n}{n} = \frac{5-\sqrt{5}}{10}$.*

It is interesting to note that the same value, $\frac{5-\sqrt{5}}{10}$, appears as the asymptotic limit of several statistics on non-decreasing Dyck paths and corresponding trees [17].

Let us now impose an additional constraint on our dissections, requiring that the endpoints of any diagonal must be separated by at least $l \geq 1$ intervening vertices. In other words, we require that each ear of the dissection [12] be at least $l+1$ edges long. Denote the number of such dissections of a convex n-gon by k totally disjoint diagonals by $D_k^{(l)}(n)$. By a reasoning similar to that in the Theorem 10, we obtain the following result.

Theorem 13 *For all $n \geq 3, 1 \leq k \leq \lfloor \frac{n-2}{2} \rfloor$ and $l \geq 1$ we have*

$$D_k^{(l)}(n) = S_k^{(l)}(n) - \sum_{m=1}^{l} m S_{k-1}^{(l)}(n-m-1).$$

Recall that the dissections of a convex n-gon by diagonals that do not intersect in its interior are counted by the little Schröder numbers s_{n-2} (sequence A001003 in [16]). We can compare asymptotic behavior of the two types of dissections.

Proposition 14

$$\frac{D_n}{s_{n-2}} \sim \sqrt{\frac{15+7\sqrt{5}}{6\sqrt{2}-8}} \left(1 - \frac{2}{n}\right)^{-3/2} \left(\frac{3+\sqrt{5}}{6+4\sqrt{2}}\right)^n.$$

Proof. Follows by comparing the asymptotics $D_n \sim S^{(1)}(n) \sim \sqrt{\frac{15+7\sqrt{5}}{8\pi}} \left(\frac{3+\sqrt{5}}{2}\right)^n n^{-3/2}$ (Proposition 2.2 of [8]) with the asymptotics for the little Schröder numbers s_n given in [16]. ■

It is also possible to think of polygon dissections in terms of polygonal clusters [6]. We say that a connected and bounded set $W \subset \mathbb{R}^2$ is a **polygonal cluster** if W is a finite union of convex polygons which are either pairwise disjoint or share a whole edge. Each polygon in a cluster is called a **cell**. The number of cells in a cluster is its **size**, and the number of edges in its boundary is its **circumference**. Borrowing a term from benzenoid chemistry, we say that a cluster is **catacondensed** if none of its vertices is shared by more than two of its cells. The minimal number of sides over all its cells is the **girth** of a given cluster. Example of a cluster is shown on Fig.8 a), and a catacondensed cluster is represented on Fig.8 b).

Proposition 15 *The number of all catacondensed polygonal clusters of size s and circumference r is $D_{s-1}(r)$. The number of all catacondensed polygonal clusters of size s with circumference r and girth at least 4 (i.e. without triangles) is $D_{s-1}^{(2)}(n)$.*

Let us present now another geometric consequence of our results on secondary structures. Consider a circle and a set of k randomly chosen chords on this circle. What is the probability that no two of them are intersecting?

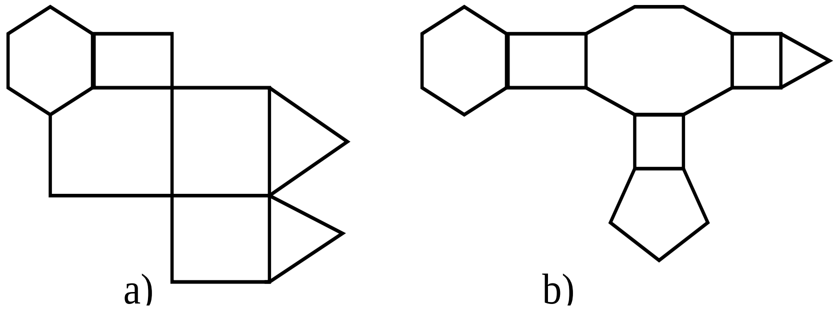

Figure 8: Examples of polygonal clusters

Proposition 16 *The probability that among k randomly chosen chords of a circle no two of them intersect is $\frac{2^k}{(k+1)!}$.*

Proof. Consider a circular representation of $K_n - E(C_n)$, where $E(C_n)$ stands for the set of edges of a cycle on n vertices. There are $\binom{\frac{n(n-3)}{2}}{k}$ k-element matchings in this graph, and any of them corresponds to a choice of a k-element subset from the set of all diagonals in a convex (regular) n-gon. Only $D_k(n)$ of such subsets are totally disjoint. Our claim follows by considering the quotient $\frac{D_k(n)}{\binom{\frac{n(n-3)}{2}}{k}}$, using Theorem 10, and letting the parameter n tend to infinity. ■

Our final geometric application of secondary structures concerns the theory of polyominoes. (We refer the reader to [10] and [13] for basic definitions and results about polyominoes.)

A **glacial landscape** of size n is a Motzkin path on n steps without peaks and trenches. The name is motivated by the resemblance of such paths to the landscapes eroded by action of glaciers; the peaks are flattened, and the trenches are widened into valleys. The set of all glacial landscapes of size n is denoted by $\mathcal{G}(n)$, and the set of all paths from $\mathcal{G}(n)$ with exactly k *Up* steps we denote by $\mathcal{G}_k(n)$. Obviously, $\mathcal{G}(n) \subset \mathcal{M}^{(1)}(n)$.

Proposition 17

$$|\mathcal{G}_k(n)| = \sum_{j=1}^{k} N(k,j) \binom{n-2j+1}{2k},$$

for all $n, k \geq 0$.

Proof. We apply the same reasoning as in the proof of Theorem 7. Namely, there are $N(k, j)$ Dyck paths on $2k$ steps with exactly j peaks (and hence with exactly $j-1$ trenches). By flattening the peaks and broadening the trenches with one *Level* step each, we get $N(k, j)$ glacial landscapes of size $2k + 2j - 1$, whose all plateaus and all valleys are exactly one step wide. Additional m *Level* steps can now be distributed in each of these landscapes in $\binom{m+2k}{2k}$ different ways. The claim now follows by denoting the total number of steps by n and summing over all $1 \leq j \leq k$. ■

Hence, $G_k(n) = |\mathcal{G}_k(n)| = \sum_{j=1}^{k} N(k, j)\binom{n-2j+1}{2k}$.

A closer look at the formula for $G_k(n)$ reveals that $G_k(n) = S_k^{(2)}(n+1)$. In a similar way one can show that $G^{(l)}(n)$, the number of all Motzkin paths on n steps whose all plateaus and valleys are at least l steps wide is equal to $\sum_k \sum_j N(k, j)\binom{n-2lj+l}{2k} = S^{(2l)}(n+l)$. The numbers $G^{(l)}(n)$ can also be interpreted as the numbers of all walks on nonnegative integers, beginning and ending at 0, with the steps $1, 0$ and -1 with **inertia** l. It means that the current direction of the walk cannot be quickly reverted.

Let us consider a glacial landscape M from $\mathcal{G}_k(n)$. Clearly, the path M has k steps of the form $(1, 1)$, and k steps of the form $(1, -1)$. Replacing these steps by the steps of the form $(0, 1)$ and $(0, -1)$, respectively, we get a lattice path P' from $(0, 0)$ to $(n - 2k, 0)$ with steps $(0, 1), (0, -1)$ and $(1, 0)$ which never falls below the x-axis. Now join the points $(0, 0)$ and $(n - 2k, 0)$ by another lattice path, starting from $(0, 0)$ by an $(0, -1)$ step, then adding $n - 2k$ steps of the form $(1, 0)$ and finally a $(0, 1)$ step to reach the point $(n-2k, 0)$. Call this path P''. The figure P enclosed between the paths P' and P'' is a polyomino with $p = n - 2k$ columns and circumference of $2r = 2n - 2k + 2$. We call the polyominoes of such shape **Manhattan polyominoes**. An example of Manhattan polyominoes with the parameters $p = 14, r = 20$ is shown on Fig.9. The set of all Manhattan polyominoes with parameters p and r we denote by $\mathcal{P}_p(r)$.

In this way to every glacial landscape from $\mathcal{G}_k(n)$ we can assign a polyomino from $\mathcal{P}_{n-2k}(n - k + 1)$. It is obvious that this mapping is injective and that we can invert it. Hence, we have

Proposition 18 *There is a bijection between* $\mathcal{G}_k(n)$ *and* $\mathcal{P}_{n-2k}(n - k + 1)$.

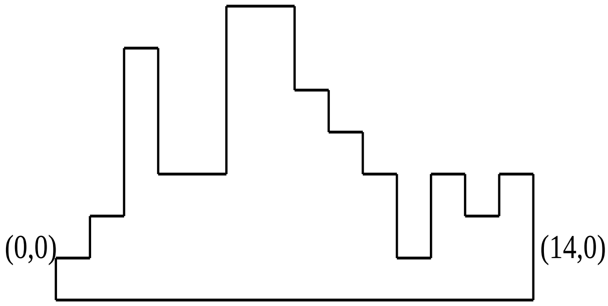

Figure 9: A Manhattan polyomino

Corollary 19 *The number of Manhattan polyominoes with* p *columns and circumference* $2r$ *is given by*

$$|\mathcal{P}_p(r)| = \sum_{j=1}^{r-p-1} N(r-p-1,j)\binom{2(r-j)-p+1}{2(r-p-1)} = S^{(2)}_{r-p-1}(2r-p-1),$$

for $r \geq p+1$*,* $p \geq 0$*.*

Reasoning in the same way as in Proposition 18, one can show that the number of all Motzkin paths of length n whose all plateaus are at least l steps long, and whose all valleys are at least m steps wide is

$$S^{(l,m)}(n) = S^{(l+m)}(n+m).$$

1.6 Concluding remarks

In this paper we have collected various results about secondary structures and pointed out several connections between them and other combinatorial families. In particular, we have used enumerative results obtained in our previous work to give explicit formulas and asymptotic behavior for sequences enumerating various classes of polygon dissections and restricted polyominoes.

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Sum-Balaban index and its properties

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Abstract

The sum-Balaban index is defined as $SJ(G) = \frac{m}{m-n+2} \sum \frac{1}{\sqrt{w(u)+w(v)}}$, where the sum is taken over all edges of a connected graph G, n and m are the cardinalities of the vertex and the edge set of G, respectively, and $w(u)$ (resp. $w(v)$) denotes the sum of distances from u (resp. v) to all the other vertices of G. In the paper known results on this recently introduced topological index are summarized.

Keywords: Balaban index, sum-Balaban index; extremal graphs; molecular descriptor

MSC: 05C12, 92E10

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1.1 Introduction

Topological indices are numerical parameters mathematically derived from the graph structure. They are widely used for establishing correlations between the structure of a molecular compound and its physico-chemical properties or biological activity. With respect to the invariant which plays a crucial role in the definition, we usually divide topological indices into three types: degree-based indices, distance-based indices and spectrum-based indices. Sum-Balaban index, the subject of this paper, is one of many distance-based topological indices.

To present its definition, we first need to introduce the basic notions. For a graph G, by $V(G)$ and $E(G)$ we denote the vertex and edge sets of G, respectively. Let $n = |V(G)|$ and $m = |E(G)|$. For vertices $u, v \in V(G)$, by $\mathrm{dist}_G(u, v)$ (or shortly just $\mathrm{dist}(u, v)$) we denote the distance from u to v in G, and by $w(u)$ we denote the *transmission* (or the *status*) of u, defined as $w(u) = \sum_{x \in V(G)} d_G(u, x)$. A predecessor of sum-Balaban index, *Balaban index* $J(G)$ of a connected graph G, defined as

$$J(G) = \frac{m}{m-n+2} \sum_{e=uv} \frac{1}{\sqrt{w(u) \cdot w(v)}},$$

was introduced in early eighties by Balaban [2, 3]. Later Balaban et al. [4] (and independently also Deng [7]) proposed a derived measure, namely the *sum-Balaban index* $\mathrm{SJ}(G)$ for a connected graph G:

$$\mathrm{SJ}(G) = \frac{m}{m-n+2} \sum_{uv \in E(G)} \frac{1}{\sqrt{w(u) + w(v)}}.$$

Since its introduction in 2010 sum-Balaban index was successfully used in QSAR/QSPR modeling, but recently it also attracted attention of mathematicians. In this paper we describe the state of the art on mathematical properties of sum-Balaban index and expose some questions, which stay unanswered.

1.2 Sum-Balaban index of trees

To avoid ambiguity we need to mention that throughout this paper we consider simple and connected graphs. In this first section we further restrict to the class of trees, which are especially interesting from the chemists point of view. Deng [7] and Xing et al. [24] considered trees with the given number of vertices.

Theorem 1 *For a tree T on $n \geq 2$ vertices, we have*

$$\mathrm{SJ}(P_n) \leq \mathrm{SJ}(T) \leq \mathrm{SJ}(S_n)$$

with left (right, respectively) equality if and only if $T = P_n$ ($T = S_n$, respectively), where P_n is the path on n vertices and S_n is the star on n vertices.

In [24] also trees with the second-largest, and third-largest (as well as the second-smallest, and third-smallest) sum-Balaban index among the n-vertex trees for $n \geq 6$ were determined. Their proof is based on specific transformations, which increase sum-Balaban index. In [19] alternative proof for the above results and tools which enabled the authors to give further ranking up to seventh maximum sum-Balaban index were presented. The results are summarized in Table 1, where T_k denotes the tree with the k-th largest sum-Balaban index. In what follows we describe the graphs mentioned in the table.

A double star $D_{a,b}$ is a tree consisting of $a + b$ vertices, two of which have degrees a and b, while the remaining ones have degree 1. By symmetry, we may assume that $a \geq b$. In Figure 1 we have the double star $D_{7,2}$.

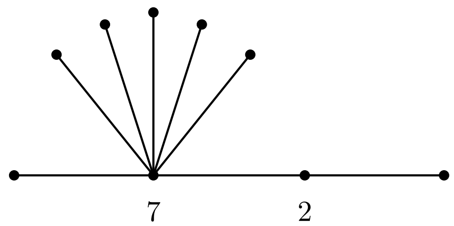

Figure 1: The double star $D_{7,2}$.

By $H_{a_1,a_2,\ldots,a_{d-1}}$ we denote a tree consisting of a diametric path of length d (i.e., with $d + 1$ vertices) and a couple of pendant edges, such that the degrees of vertices of the diametric path are $1, a_1, a_2, \ldots, a_{d-1}, 1$. That is, $H_{a_1,a_2,\ldots,a_{d-1}}$ is a *caterpillar*. Due to symmetry, we may assume that $a_1 \geq a_{d-1}$ in $H_{a_1,a_2,\ldots,a_{d-1}}$, see Figure 2 for $H_{3,7,2}$.

Let $n \geq 7$. By R_n we denote the graph obtained from a star on $n - 3$ vertices by subdividing three distinct edges, see Figure 3 for R_{11}.

It was also observed in [19] that for every k, the value $\mathrm{SJ}(T_1) - \mathrm{SJ}(T_k)$ is tending to $c_k\sqrt{n}$, where c_k is a constant depending on k but not on n.

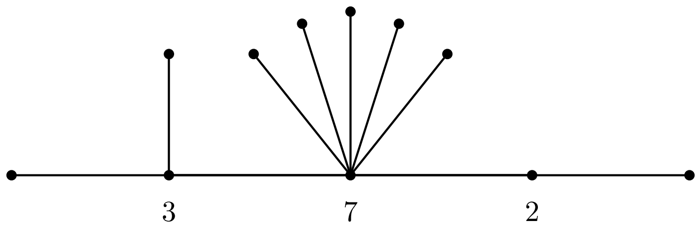

Figure 2: A caterpillar $H_{3,7,2}$.

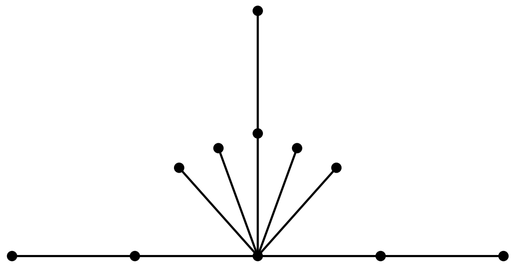

Figure 3: The graph R_{11}.

For the maximum value of sum-Balaban index for trees with given diameter the interested reader is referred to [26].

1.3 Extremal values for n-vertex graphs

In [24] various upper and lower bounds are given for graphs with given parameters such as the maximum degree, number of edges, etc. The authors considered also the special case of bipartite graphs. However, in this section we are interested in extremal values of sum-Balaban index in the case when only the number of vertices is prescribed.

1.3.1 Maximum values

The *cyclomatic number* μ of G, which is the minimum number of edges that must be removed from G in order to transform it to an acyclic graph, equals $m-n+1$. Note that the denominator $m-n+2$ in the definition of Balaban and sum-Balaban index

<table>
<tr><th>n</th><th>T_1</th><th>T_2</th><th>T_3</th><th>T_4</th><th>T_5</th><th>T_6</th><th>T_7</th></tr>
<tr><td>$2-3$</td><td rowspan="10">S_n</td><td></td><td rowspan="2"></td><td rowspan="3"></td><td rowspan="3"></td><td rowspan="3"></td><td rowspan="4"></td></tr>
<tr><td>4</td><td rowspan="9">$D_{n-2,2}$</td></tr>
<tr><td>5</td><td>P_5</td></tr>
<tr><td>6</td><td rowspan="7">$D_{n-3,3}$</td><td rowspan="2">$H_{2,n-3,2}$</td><td rowspan="2">$H_{n-3,2,2}$</td><td>P_6</td></tr>
<tr><td>7</td><td>$H_{3,3,2}$</td><td>R_7</td></tr>
<tr><td>8</td><td>$D_{4,4}$</td><td>$H_{2,5,2}$</td><td rowspan="2">$H_{n-3,2,2}$</td><td rowspan="2">$H_{3,n-4,2}$</td></tr>
<tr><td>9</td><td rowspan="4">$H_{2,n-3,2}$</td><td rowspan="3">$D_{n-4,4}$</td></tr>
<tr><td>$10-11$</td><td>$D_{n-5,5}$</td><td>$H_{n-3,2,2}$</td></tr>
<tr><td>$12-22$</td><td>$H_{n-3,2,2}$</td><td rowspan="2">$H_{3,n-4,2}$</td></tr>
<tr><td>$23-\infty$</td><td>$H_{n-3,2,2}$</td><td>$D_{n-4,4}$</td></tr>
</table>

Table 1: First seven trees with maximal values of sum-Balaban index.

can be expressed as $\mu + 1$. In [20] n-vertex graphs which contain at least one cycle were considered.

Theorem 2 *Let G be a connected graph on n vertices with $\mu \geq 1$. Then $\mathrm{SJ}(G)$ is maximum if and only if G is the complete graph K_n.*

In [21] we found an erroneous statement that complete graphs attain the maximum sum-Balaban index among all n-vertex graphs. However this is true only for small cases of n as proved in [20].

Theorem 3 *For any connected graph G on $n \geq 2$ vertices, we have*

$$\mathrm{SJ}(G) \leq \begin{cases} \mathrm{SJ}(K_n), & \text{if } n \leq 5 \\ \mathrm{SJ}(S_n), & \text{if } n \geq 6. \end{cases}$$

Moreover, the next theorem implies that for every k and large enough n, the first k graphs of order n with the largest value of Balaban index are trees [20].

Theorem 4 *Let a and b be positive integers such that $a, b \geq 2$, $a + b = n$ and $n \geq 8$. Then $\mathrm{SJ}(D_{a,b}) > \mathrm{SJ}(K_n)$.*

One can observe that Theorems 2 and 3 imply the following:

Corollary 5 *Let G be a graph with the maximum value of sum-Balaban index in the class of k-connected (k-edge-connected) graphs of order n. Then we have:*

(1) if $k = 1$ and, $n = 2$ or $n \geq 6$, then G is the star S_n;

(2) if $k = 1$ and $n \leq 5$, or $k \geq 2$, then G is the complete graph K_n.

1.4 Minimum values

As in the case of Balaban index (see [13]) finding the minimum value of sum-Balaban index among n-vertex graphs is far more complicated problem. It remains open, however, some insight in the structure of potential candidates was given in [14]. There we have the following results.

Theorem 6 *Let G be a graph on n vertices, $n \geq 4$. Then*

$$\mathrm{SJ}(G) \geq 2\sqrt{\frac{n}{n-1}}\,.$$

It turns out that for large values of n a better lower bound on the sum-Balaban index can be obtained.

Theorem 7 *Let G be a graph on n vertices, where n is big enough. Then*

$$\mathrm{SJ}(G) \geq 4 + o(1).$$

Let K_a and $K'_{a'}$ be two disjoint complete graphs on a and a' vertices, respectively. We always assume $a \leq a'$. Further, let P_b be a path on b vertices $(v_0, v_1, \ldots, v_{b-1})$ disjoint from the cliques. The *dumbbell graph* $D^0_{a,b,a'}$ is obtained from $K_a \cup P_b \cup K'_{a'}$ by joining all vertices of K_a with v_0 and all vertices of $K'_{a'}$ with v_{b-1}. Thus, $D^0_{a,b,a'}$ has $a + b + a'$ vertices. In the case when $a = a'$, we call a graph a *balanced dumbbell graph* and we denote it by $B_{a,b}$. A *dumbbell-like graph*, $D^\ell_{a,b,a'}$, is obtained from the dumbbell graph $D^0_{a,b,a'}$ by either inserting ℓ edges between v_1 and K_a if $\ell > 0$, or by removing $-\ell$ edges between v_{b-1} and $K'_{a'}$ if $\ell < 0$.

In Figure 4 one can find graphs which attain the minimum value of sum-Balaban index among n-vertex graphs where $n \leq 10$ (we remark that by removing dotted edges we obtain the corresponding graphs with the minimum value of Balaban index). Observe

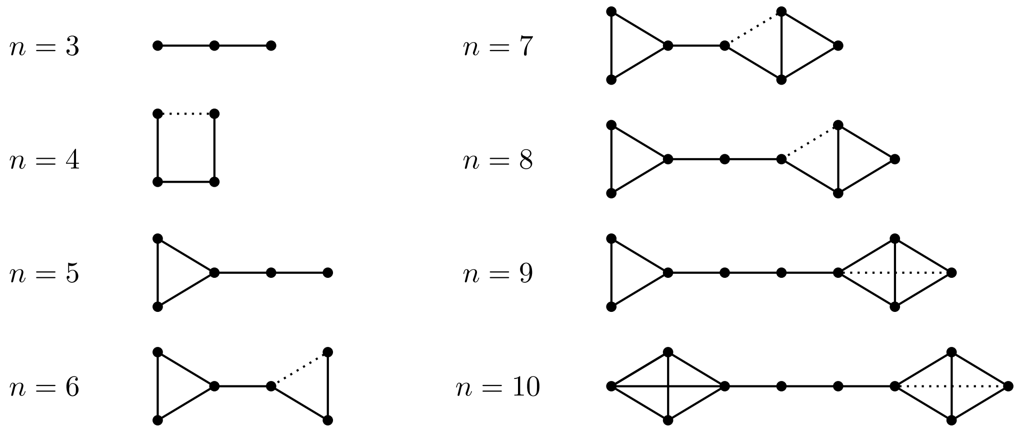

Figure 4: Graphs with the smallest value of sum-Balaban index for $n \in \{3, 4, \ldots, 10\}$.

that all graphs in Figure 4 (with the exception of the case $n = 4$) are dumbbell or dumbbell-like.

In the special case of balanced dumbbell graphs the following statement was obtained in [14].

Theorem 8 *Let $B_{a,b}$ be a balanced dumbbell graph on n vertices with the smallest possible value of sum-Balaban index. Then a and b are asymptotically equal to $\sqrt[4]{\sqrt{2}\log\left(1+\sqrt{2}\right)}\sqrt{n}$ and n, respectively. That is, $a = \sqrt[4]{\sqrt{2}\log\left(1+\sqrt{2}\right)}\sqrt{n} + o(\sqrt{n})$ and $b = n - o(n)$.*

Corollary 9 *Let B be a balanced dumbbell graph on n vertices, where n is big enough, with the minimum value of sum-Balaban index. Then*

$$\mathrm{SJ}(B) \doteq 4.47934.$$

Comparing Corollary 9 with the lower bound presented in Theorem 7, we see that the asymptotic value of sum-Balaban index for optimum balanced dumbbell graph is only about 1.12 times higher. Hence it can be expected that the optimal balanced dumbbell graph is not much different from the optimal dumbbell graph.

Conjecture 10 *Among all dumbbell graphs $D^0_{a,b,a'}$ on at least 14 vertices, the minimum value of sum-Balaban index is achieved for one with $a' = a$ or $a' = a + 1$.*

More generally, the following was conjectured in [14].

Conjecture 11 *Dumbbell-like graphs $D^\ell_{a,b,a'}$ attain the minimum value of sum-Balaban index.*

1.5 Accumulation points of sum-Balaban index

In [18] it is shown that for every nonnegative real number r there exists a sequence of graphs $\{G_{r,i}\}_{i=1}^{\infty}$ such that the number of vertices of $G_{r,i}$ tends to infinity as $i \to \infty$ and $\lim_{i\to\infty} J(G_{r,i}) = r$. An analogous result was proved for sum-Balaban index [20]. Denote $Q = \sqrt{2}\ln(1+\sqrt{2})$. Observe that $Q \doteq 1.24650$ and $1+Q+2\sqrt{Q} \doteq 4.47934$. We have the following statement.

Theorem 12 *Let $r \geq 1 + Q + 2\sqrt{Q}$. Further, let $\{B_{a_i,b_i}\}_{i=1}^{\infty}$ be a sequence of balanced dumbbell graphs on $n_i = 2a_i + b_i$ vertices such that $n_i \to \infty$ and*

$$\lim_{i\to\infty} \frac{a_i}{\sqrt{n_i}} = \frac{1}{\sqrt{2}}\sqrt{r - 1 - Q + \sqrt{(r-1-Q)^2 - 4Q}}.$$

Then $\lim_{i\to\infty} \mathrm{SJ}(B_{a_i,b_i}) = r$.

Although we conjecture that for graphs G on large number of vertices $\mathrm{SJ}(G) \geq 1+Q+2\sqrt{Q}$ (see Corollary 9), it is proved only that $\mathrm{SJ}(G) \geq 4 + o(1)$ (see Theorem 7). Hence, if the conjecture is false, then the problem of accumulation points of sum-Balaban index for values in the interval $[4, 4.47934)$ remains open.

1.6 Unicyclic and bicyclic graphs

Unicyclic graphs on n vertices with the maximum sum-Balaban index were considered in [25]. Let S_n^+ denote the graph, obtained from the star S_n by adding an edge between two nonadjacent vertices of the star.

Theorem 13 *Let G be a connected unicyclic graph on $n \geq 4$ vertices. Then*

$$\mathrm{SJ}(G) \leq \frac{n}{2}\left(\frac{1}{\sqrt{4n-8}} + \frac{2}{\sqrt{3n-5}} + \frac{n-3}{\sqrt{3n-4}}\right),$$

where the equality holds if and only if $G = S_n^+$.

A connected graph on n vertices is said to be *bicyclic* if it contains exactly $n+1$ edges. Denote by S_n^{++} the bicyclic graph obtained from the star S_n by adding two edges with a common vertex (see Figure 5 where S_7^{++} is depicted).

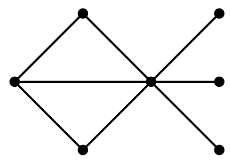

Figure 5: The graph S_7^{++}.

Maximum values of sum-Balaban index were first examined in [6]. However, Fang et al. [11] found some flaws in this paper and proved the following.

Theorem 14 *The graph S_n^{++} has the largest sum-Balaban index among all n-vertex bicyclic graphs.*

1.7 Regular graphs

Folowing the results of [15], Lei et al. [21] proved that for an r-regular graph G on n vertices with $r \geq 3$ it holds

$$\mathrm{SJ}(G) \leq \frac{r^2(r-1)n^{\frac{1}{2}}}{2(r-2)^{\frac{3}{2}}\sqrt{2\left\lfloor \log_{r-1}\left(\frac{(r-2)n+2}{r}\right)\right\rfloor}}.$$

They also considered fullerenes, and proved that if they contain at least 60 vertices, then $\mathrm{SJ}(G) \leq \frac{9n}{\sqrt{n\sqrt{n}}}$.

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Weighted Lattice Paths Enumeration by Gaussian Polynomials

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Abstract

The Gaussian polynomial in variable q is defined as the q-analog of the binomial coefficient. In addition to remarkable implications of these polynomials to abstract algebra, matrix theory and quantum computing, there is also a combinatorial interpretation through weighted lattice paths. This interpretation is equivalent to weighted board tilings, which can be used to establish Gaussian polynomial identities. In particular, we prove duals of such identities and evaluate related sums.

Keywords: Gaussian binomial coefficient, q-binomial coefficient, Gaussian polynomial identities, q-analog, lattice paths, domino tiling, double counting

MSC: 05A30, 11B65

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1.1 Introduction

We let n and k denote non-negative integers. The *Gaussian polynomial* or *q-binomial coefficient* is defined to be

$$\begin{bmatrix} n \\ k \end{bmatrix}_q = \frac{(q^n-1)(q^{n-1}-1)\cdots(q^{n-k+1}-1)}{(q^k-1)(q^{k-1}-1)\cdots(q-1)}.$$

Thus, we replace each factor m in the formula for binomial coefficient, by q^m-1 to get Gaussian coefficient. It is easily seen that Gaussian binomial coefficient reduces to binomial coefficient when $q=1$. More precisely, by the L'Hôpital's Rule, we have

$$\lim_{q\to 1}\begin{bmatrix} n \\ k \end{bmatrix}_q = \binom{n}{k}.$$

More on this subject one can find in the book by P. Cameron [3]. Recall a classical implication of Gaussian polynomial. The number of elements in a finite field is a prime power and up to isomorphism there is a unique field of any prime power order (E. Galois). We let GF(q) denote the field with q elements. Then the number of k-dimensional subspaces of an n-dimensional vector space over GF(q) is $\left[\begin{smallmatrix} n \\ k \end{smallmatrix}\right]_q$. A proof of this one can find in a nice overview by H. Cohn [4]. It is also worth mentioning that Gaussian polynomial are related to *quantum calculus* and more on this one can find in a book by V. Kac and P. Cheung [7].

Having the q-analog of the factorial defined as

$$[n]_q! = (1+q)(1+q+q^2)\cdots(1+q+\cdots+q^{n-1})$$

we also have

$$\begin{bmatrix} n \\ k \end{bmatrix}_q = \frac{[n]_q!}{[k]_q![n-k]_q!}.$$

Recently, V. Guo and D. Yang [5] found Gaussian polynomial identities

$$\begin{aligned}
\sum_{k=0}^{\lfloor n/2\rfloor}\begin{bmatrix} m+k \\ k \end{bmatrix}_{q^2}\begin{bmatrix} m+1 \\ n-2k \end{bmatrix}_q q^{\binom{n-2k}{2}} &= \begin{bmatrix} m+n \\ n \end{bmatrix}_q, \\
\sum_{k=0}^{\lfloor n/4\rfloor}\begin{bmatrix} m+k \\ k \end{bmatrix}_{q^4}\begin{bmatrix} m+1 \\ n-4k \end{bmatrix}_q q^{\binom{n-4k}{2}} &= \sum_{k=0}^{\lfloor n/2\rfloor}(-1)^k\begin{bmatrix} m+k \\ k \end{bmatrix}_{q^2}\begin{bmatrix} m+n-2k \\ n-2k \end{bmatrix}_q
\end{aligned}$$

which are q-analogues of binomial coefficient identities of Y. Sun,

$$\begin{aligned}\sum_{k=0}^{\lfloor n/2\rfloor}\binom{m+k}{k}\binom{m+1}{n-2k} &= \binom{m+n}{n},\\ \sum_{k=0}^{\lfloor n/4\rfloor}\binom{m+k}{k}\binom{m+1}{n-4k} &= \sum_{k=0}^{\lfloor n/2\rfloor}(-1)^k\binom{m+k}{k}\binom{m+n-2k}{m},\end{aligned}$$

respectively. (For an overview of binomial coefficients we refer the reader to classical reference by R. Graham, D. Knuth and O. Patashnik [6].) Being motivated by these results, in this work we aim at finding further Gaussian polynomial identities.

1.2 q-binomial coefficients and weighted lattice paths

As the basic recurrences for Gaussian polynomials we have

$$\begin{bmatrix} n \\ k \end{bmatrix}_q = \begin{bmatrix} n-1 \\ k-1 \end{bmatrix}_q + q^k \begin{bmatrix} n-1 \\ k \end{bmatrix}_q \tag{1}$$

and

$$\begin{bmatrix} n \\ k \end{bmatrix}_q = q^{n-k}\begin{bmatrix} n-1 \\ k-1 \end{bmatrix}_q + \begin{bmatrix} n-1 \\ k \end{bmatrix}_q \tag{2}$$

where $0 < k < n$ and

$$\begin{bmatrix} n \\ 0 \end{bmatrix}_q = \begin{bmatrix} n \\ n \end{bmatrix}_q = 1.$$

This follows immediately from the definition. To prove (1) we have

$$\begin{aligned}\begin{bmatrix} n \\ k \end{bmatrix}_q - \begin{bmatrix} n-1 \\ k-1 \end{bmatrix}_q &= \left(\frac{q^n-1}{q^k-1}-1\right)\begin{bmatrix} n-1 \\ k-1 \end{bmatrix}_q\\ &= q^k\left(\frac{q^{n-k}-1}{q^k-1}\right)\begin{bmatrix} n-1 \\ k-1 \end{bmatrix}_q\\ &= q^k\begin{bmatrix} n \\ k-1 \end{bmatrix}_q.\end{aligned}$$

In the same fashion one can prove the property of *symmetry* for Gaussian polynomials,

$$\begin{bmatrix} n \\ k \end{bmatrix}_q = \begin{bmatrix} n \\ n-k \end{bmatrix}_q \tag{3}$$

as well as an analogy of the property of *absorption* for binomial coefficients,

$$\begin{bmatrix} n \\ k \end{bmatrix}_q = \frac{1-q^n}{1-q^{n-k}} \begin{bmatrix} n-1 \\ k-1 \end{bmatrix}_q . \tag{4}$$

A well known combinatorial interpretation of Gaussian polynomial $\left[\begin{smallmatrix} n \\ k \end{smallmatrix}\right]_q$ is that it enumerates the number of *integer partitions* that fit into the *square lattice* region of size $k \times (n-k)$ (see the book [2] by J. Azose, A. Benjamin and K. Garrett). More precisely, the Gaussian polynomial can be defined as the *generating function* for this type of partitions. For example, consider the polynomial

$$\begin{bmatrix} 4 \\ 2 \end{bmatrix}_q = q^4 + q^3 + 2q^2 + q + 1.$$

This means that there are six distinct partitions whose *Young diagrams* fit into a 2×2 lattice region and that these partitions are

$$(2,2), (2,1), (2), (1,1), (1), (0)$$

(there are 2 partitions of the number 2 while the other partitions are of numbers 4, 3, and 1. Now the symmetry property (3) follows immediately by conjugation of the Young diagrams. Similar bijective proofs can also be done for recurrences (1) and (2) (see the book [1] by G. Andrews and K. Ericcson).

Obviously, instead by partitions, one can interpret Gaussian polynomial by lattice paths from $(0,0)$ to $(k, n-k)$, where an increment by 1 right has the weight of 1 while an increment by 1 up has the weight of q^s where s is the number of previous horizontal increments. Furthermore, we establish a bijection between these paths and a *board tilings* by squares and dominoes as follows:

i) we code an increment by 1 right in a path by a domino, and

ii) we code an increment by 1 up by a square.

We illustrate this 1 to 1 correspondence in Figure 1. The reasoning above proves the next lemma.

Lemma 1 *The Gaussian polynomial* $\left[{n \atop k}\right]_q$ *represents the number of* $(n+k)$*-board tilings by* $n-k$ *squares and* k *dominoes where the weight of every domino is equal to 1 while the weight of a square is equal to* q^s*, with* s *being the number of preceding dominoes.*

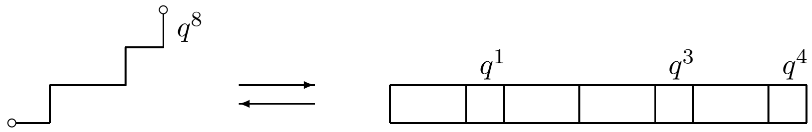

Figure 1: There is a 1 to 1 correspondence between weighted lattice paths with k horizontal increments and weighted board tilings with k dominoes.

Note that the parameter n in Lemma 1 represents the number of parts in a tiling (the number of increments of length 1 in a lattice path). Figure 2 shows 6-board tilings that correspond to partitions in the example above. According to Lemma 1, these tilings are represented by the Gaussian polynomial $\left[{4 \atop 2}\right]_q$. In what follows we use Lemma 1 to prove some Gaussian polynomial identities.

Figure 2: All six tilings of a board of length 6 having two dominoes, which are enumerated by the polynomial $q^4+q^3+2q^2+q+1$.

1.3 Two pairs of polynomial identities

We shall now present obtained identities for the Gaussian polynomials, in the following statements. To get these, we enumerate elements of the set of all n-board weighted tilings in respect to certain criterions.

Theorem 1 *For natural numbers* n *and* k*, where* $n \geq k$*, we have*

$$\sum_{i=0}^{k} q^i \begin{bmatrix} n-k-1+i \\ i \end{bmatrix}_q = \begin{bmatrix} n \\ k \end{bmatrix}_q .$$

Proof. We consider weighted $(n+k)$-board tilings with k dominoes and $n-k$ squares, in respect to the last square in a tiling. The set S of all such tilings we separate into k disjoint subsets $S_1, S_2, \ldots, S_k$ such that in set S_1 there are tilings having the last square on the position $n+k-1$. In S_2 there are tilings having the last square on position $n+k-3$ (meaning that there are $k-1$ dominoes left from the last square and a sole domino is placed right from the last square). Furthermore, in S_3 the last square is on position $n+k-5$, etc.

Now, the tilings in S_1 are represented by

$$\begin{bmatrix} n-1 \\ k \end{bmatrix}_q q^k.$$

Namely, by Lemma 1, tilings of the length $n+k-1$ are represented by $\left[\begin{smallmatrix} n-1 \\ k \end{smallmatrix}\right]_q$ and the weight of the last square is q^k (since there are k dominoes placed on the left of the last square). Furthermore, by an analogue argument, tilings in S_2 are represented by

$$\begin{bmatrix} n-2 \\ k-1 \end{bmatrix}_q q^{k-1},$$

etc. Finally, tilings in the set S_k are represented by

$$\begin{bmatrix} n-k-1 \\ 0 \end{bmatrix}_q,$$

since there are no dominoes on the left of the last square. Having in mind that the sets S_i are disjoint, the sum

$$\begin{bmatrix} n-1 \\ k \end{bmatrix}_q q^k + \begin{bmatrix} n-2 \\ k-1 \end{bmatrix}_q q^{k-1} + \cdots + \begin{bmatrix} n-k-1 \\ 0 \end{bmatrix}_q$$

represents the set S and this fact completes the proof.

■

For the purpose of proving the following theorem, again we consider weighted $(n+k)$-board tilings with k dominoes and $n-k$ squares, but now with respect to the last domino in a tiling.

Theorem 2 *For natural numbers n and k, where $n \geq k$, we have*

$$\sum_{i=0}^{n-k} q^{k(n-k-i)} \begin{bmatrix} k-1+i \\ k-1 \end{bmatrix}_q = \begin{bmatrix} n \\ k \end{bmatrix}_q.$$

Proof. The set S of weighted tilings of length $n+k$ we decompose into partition of $n-k+1$ disjoint subsets $S_0, S_1, S_2, \dots, S_{n-k}$, such that in the subset S_i there are exactly $n-k-i$ squares on the right hand side of the last domino in a tiling.

The set S_0 is represented by

$$\begin{bmatrix} k-1 \\ k-1 \end{bmatrix}_q q^{k(n-k)}.$$

This holds true since on the left hand side from the last domino in S_0 there are $k-1$ dominoes and from the fact that there are $n-k$ squares on the right hand side of the last domino - in every of these tilings. Tilings in the set S_1 have $n-r-1$ dominoes on the right hand side of the last domino which means that they are enumerated by

$$\begin{bmatrix} k \\ k-1 \end{bmatrix}_q q^{k(n-k-1)},$$

etc. Finally, tilings in the set S_{n-k} are represented by the polynomial

$$\begin{bmatrix} n-1 \\ k-1 \end{bmatrix}_q.$$

Thus, the sum of these terms,

$$\begin{bmatrix} k-1 \\ k-1 \end{bmatrix}_q q^{k(n-k)} + \begin{bmatrix} k \\ k-1 \end{bmatrix}_q q^{k(n-k-1)} + \cdots + \begin{bmatrix} n-1 \\ k-1 \end{bmatrix}_q$$

is equal to the polynomial $\left[\begin{smallmatrix} n \\ k \end{smallmatrix}\right]_q$. ∎

Figure 3 shows tilings of length 7 with two dominoes and three squares separated into subsets S_0, S_1, S_2, S_3, with respect to the last domino. One can easily establish that $|S_0| = 1, |S_1| = 2, |S_2| = 3, |S_3| = 4$ and that polynomial $\left[\begin{smallmatrix} 5 \\ 2 \end{smallmatrix}\right]_q$ enumerates these tilings.

In order to prove Theorem 3 we consider a class of tilings with an odd number of dominoes. More precisely, we take into account weighted $(n+2r+1)$-board tilings with $2r+1$ dominoes. The set S of all such tilings we separate into $n-2r$ subsets $S_1, S_2, \dots, S_{n-2r}$, by means of the median domino. Tilings in set S_i have the median domino covering cells $2r+i$ and $2r+i+1$. Thus, in S_1 there are tilings having the median domino covering cells $2r+1$ and $2r+2$. This means that on the left hand side of the median domino there are r dominoes covering cells 1 through $2r$. Now we separate a tiling into parts t_1 - from cells 1 through $2r$ and t_2 - from cells $2r+3$ through $n+2r+1$.

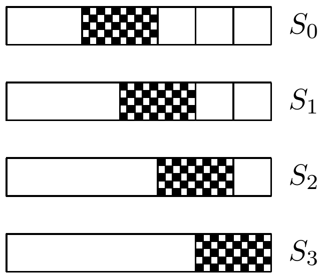

Figure 3: Tilings of length 7 with two dominoes and three squares separated into four subsets, with respect to the last domino in a tiling.

Clearly, the tilings in the set t_1 are enumerated by $\left[{r \atop r}\right]_q$. The tilings in t_2 are enumerated by

$$\begin{bmatrix} n-r-1 \\ r \end{bmatrix}_q q^{(r+1)(n-2r-1)},$$

where the factor $q^{(r+1)(n-2r-1)}$ is added because there are $r+1$ dominoes left from a tiling in t_2 and there are $n-2r-1$ squares in a such tiling. By the same arguments one can conclude that the tilings in S_2 are enumerated by the polynomial

$$\begin{bmatrix} r+1 \\ r \end{bmatrix}_q \begin{bmatrix} n-r \\ r \end{bmatrix}_q q^{(r+1)(n-2r-2)},$$

tilings in S_3 by

$$\begin{bmatrix} r+2 \\ r \end{bmatrix}_q \begin{bmatrix} n-r+1 \\ r \end{bmatrix}_q q^{(r+1)(n-2r-3)},$$

$\dots$, and tilings in S_{n-2r} by

$$\begin{bmatrix} n-r-1 \\ r \end{bmatrix}_q \begin{bmatrix} r \\ r \end{bmatrix}_q .$$

Finally, these terms sum up to

$$\begin{bmatrix} r \\ r \end{bmatrix}_q \begin{bmatrix} n-r-1 \\ r \end{bmatrix}_q q^{(r+1)(n-2r-1)} + \dots + \begin{bmatrix} n-r-1 \\ r \end{bmatrix}_q \begin{bmatrix} r \\ r \end{bmatrix}_q$$

which is the polynomial $\left[{n \atop 2r+1}\right]_q$. This reasoning completes the proof of Theorem 3.

Theorem 3 *For natural numbers n and r, where $n \geq 2r+1$, we have*

$$\sum_{i=1}^{n-2r} q^{(r+1)(n-2r-i)} \begin{bmatrix} r-1+i \\ r \end{bmatrix}_q \begin{bmatrix} n-r-i \\ r \end{bmatrix}_q = \begin{bmatrix} n \\ 2r+1 \end{bmatrix}_q .$$

As an illustration of Theorem 3 we can take that there are 20 tilings of the length 9, tiled by three dominoes and three squares. These can be separated by means of the median domino into sets S_1, S_2, S_3 and S_4, where $|S_1| = 4, |S_2| = 6, |S_3| = 6, |S_4| = 4$ (Figure 4). These cardinalities correspond to the terms in the equality stated in Theorem 3 for $n = 6$ and $r = 1$. The Gaussian polynomial $\begin{bmatrix} 6 \\ 3 \end{bmatrix}_q$ representing these tilings reads as

$$q^9 + q^8 + 2q^7 + 3q^6 + 3q^5 + 3q^4 + 3q^3 + 2q^2 + q + 1.$$

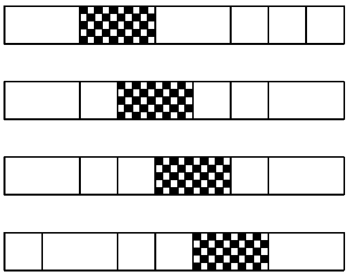

Figure 4: Representatives of sets $S_1, \ldots, S_4$, respectively, of tilings of length 9 with three dominoes, with the central domino marked.

Having in mind the symmetry of pairs of factors under the sum in Theorem 3, we have a simple consequence to binomial coefficients. By the substitution $m = n - 2r$ we immediately obtain the following corollary.

Corollary 1 *For natural numbers n and r, where n is even we have*

$$2 \sum_{i=1}^{n/2} \binom{r-1+i}{r} \binom{n+r-i}{r} = \binom{n+2r}{2r+1}.$$

In order to prove our next result, we consider the class of $(n+r)$-board tilings having r dominoes where the constraint on the length of a tiling is that $n-r$ must be odd.

Thus, the number of squares in a tiling is odd which provides us a double counting of tilings. By Lemma 1, the coefficient $\begin{bmatrix} n \\ r \end{bmatrix}_q$ enumerates these tilings. On the other hand, the sum

$$\begin{bmatrix} \frac{n-r-1}{2} \\ 0 \end{bmatrix}_q \begin{bmatrix} \frac{n-r-1}{2}+r \\ k \end{bmatrix}_q + \begin{bmatrix} \frac{n-r-1}{2}+1 \\ 1 \end{bmatrix}_q \begin{bmatrix} \frac{n-r-1}{2}+r-1 \\ k-1 \end{bmatrix}_q q^{(n-r+1)/2} + \cdots + \begin{bmatrix} \frac{n-r-1}{2}+r \\ k \end{bmatrix}_q \begin{bmatrix} \frac{n-r-1}{2} \\ 0 \end{bmatrix}_q q^{r(n-r+1)/2}$$

consisting of $r+1$ terms also enumerates them. This follows by analogue arguments as in the previous proof, with the difference that here we enumerate tilings with respect to the median square (which always exists since their number is odd). Now, by the substitution $m := n-r$, we have the following statement.

Theorem 4 *For natural numbers n and r, where n is odd, we have*

$$\sum_{i=0}^{r} q^{i(n+1)/2} \begin{bmatrix} \frac{n-1}{2}+i \\ i \end{bmatrix}_q \begin{bmatrix} \frac{n-1}{2}+r-i \\ r-i \end{bmatrix}_q = \begin{bmatrix} n+r \\ r \end{bmatrix}_q .$$

In the same fashion as in case of Theorem 3 we consider, as an illustration of Theorem 4, tilings of the length 13. The Gaussian polynomial $\begin{bmatrix} 9 \\ 4 \end{bmatrix}_q$ representing these tilings reads as

$$q^{20}+q^{19}+2q^{18}+3q^{17}+5q^{16}+6q^{15}+8q^{14}+9q^{13}+11q^{12}+11q^{11}+ 12q^{10}+11q^{9}+11q^{8}+9q^{7}+8q^{6}+6q^{5}+5q^{4}+3q^{3}+2q^{2}+q+1.$$

Again we have a consequence to binomial coefficients and we state it in Corollary 2.

Corollary 2 *For odd natural numbers n and r we have*

$$2\sum_{i=0}^{(r+1)/2} \binom{\frac{n-1}{2}+i}{i} \binom{\frac{n-1}{2}+r-i}{r-i} = \binom{n+r}{r}.$$

1.4 Concluding remarks

In this paper we use a combinatorial interpretation of q-binomial coefficients through the weighted lattice paths to establish identities for these polynomials. In particular, we establish two duals of Gaussian polynomial identities. A pair of identities is stated in Theorems 1 and 8. In Theorems 3 and 4 we evaluate the sum with terms of two factors.

We believe that ideas and results presented here could be used to get further Gaussian polynomial identities. Here we enumerate weighted tilings with respect to position of the last square, the last domino, the median domino and the median square. We are fairly convinced that one can found other similar criteria and employ them to obtain further identities. More refined constraints on tilings could possibly lead to even more interesting relations for Gaussian polynomials.

Acknowledgement

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An Invitation to Combinatorial Tropical Geometry

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Abstract

This paper addresses an overview on the recent development of the area known as the tropical geometry. In particular we point out combinatorial aspect of the field. After a brief introduction to tropical algebra we discuss tropical hypersurfaces and applications in enumerative geometry.

Keywords: tropical geometry, tropical curve, Gromov-Witten invariant, Newton subdivision

MSC: 14A99, 14N10, 14T05, 52B20

1.1 Introduction

The *tropical geometry* is a very new area in mathematics, that is in essence closely related to algebraic geometry. While rapid development of the area begins with this century, its leading ideas had appeared in earlier works of G. M. Bergman and others. Recent significant contribution to the theory has been made by G. Mikhalkin in particular within the paper that can be understand as foundation of *enumerative algebraic geometry* (see [17, 18, 19, 21]).

It is worth mentioning that the attribute "tropical" has no any intuitive meaning related to the theory but was coined by French mathematicians in honor of the Brazilian

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mathematician Imre Simon, who contributes to the field [24]. In what follows we are firstly concerned with tropical arithmetic and its relations to classical arithmetic. Then we give an example of tropical geometry and combinatorial mathematics. Besides we define tropical curves and correlation with enumerative algebraic geometry.

We also presents recent results of Maclagan and Sturmfels (see [16]) and Mikhalkin (see [19]). For further introduction to tropical geometry one can look at references [2, 6, 10, 14, 23, 25, 26, 27]. A more advanced reader may refer to [3, 15, 20].

As an introduction to the field we present basic ideas and facts of *tropical algebra*. The set of *tropical numbers* is defined as $\mathbb{T} = \mathbb{R} \cup \{\infty\}$ whereas operations of *tropical addition* and *multiplication* on $\mathbb{T}$ are defined as

$$x \oplus y := \min(x, y)$$

$$x \odot y := x + y,$$

with the usual conventions when one of the operands is ∞ [16]. For example, we have $3 \oplus 5 = 3$, $3 \odot 5 = 8$. The set $\mathbb{T}$ equipped with these operations form a *tropical semiring* $(\mathbb{R}, \oplus, \odot)$ or the min-plus algebra. In this triple one can replace the operation of minimum by maximum to get the isomorphic max-plus algebra. Many of axioms from arithmetic remain also in tropical algebra. As it is the case in classical algebra, we abbreviate multiplication $x \odot y$ by xy.

Having in mind that zero is the neutral element in respect to multiplication, for the coefficients in Pascal triangle we have

$$\begin{array}{ccccccccc}
 & & & & 0 & & & & \\
 & & & 0 & & 0 & & & \\
 & & 0 & & 0 & & 0 & & \\
 & 0 & & 0 & & 0 & & 0 & \\
0 & & 0 & & 0 & & 0 & & 0 \\
\cdots & \cdots & & \cdots & & \cdots & & \cdots & \cdots
\end{array}$$

When applying the binomial theorem on the third row of the triangle we get

$$(x \oplus y)^3 = (x \oplus y) \odot (x \oplus y) \odot (x \oplus y) = 0 \odot x^3 \oplus 0 \odot x^2 y \oplus 0 \odot x y^2 \oplus 0 \odot y^3 = x^3 \oplus x^2 y \oplus x y^2 \oplus y^3$$

and furthermore

$$(x \oplus y)^3 = x^3 \oplus y^3.$$

Clearly, in classical arithmetic we have

$$3 \cdot \min\{x, y\} = \min\{3x, 2x + y, x + 2y, 3y\} = \min\{3x, 3y\}$$

for every $x, y \in \mathbb{R}$. A simple generalization of this statement give as a tropical version of the binomial theorem,

$$(x \oplus y)^n = x^n \oplus y^n,\ n \in \mathbb{N}. \tag{5}$$

Over the tropical semiring, we can define a linear algebra operations of adding and multiplying vectors and matrices in the usual way. For instance,

$$\begin{pmatrix} 0 & 1 \\ 2 & 3 \end{pmatrix} \odot \begin{pmatrix} 4 & 5 \\ 6 & 7 \end{pmatrix} = \begin{pmatrix} 0 \odot 4 \oplus 1 \odot 6 & 0 \odot 5 \oplus 1 \odot 7 \\ 2 \odot 4 \oplus 3 \odot 6 & 2 \odot 5 \oplus 3 \odot 7 \end{pmatrix} = \begin{pmatrix} 4 & 5 \\ 6 & 7 \end{pmatrix}.$$

We let $x_1, x_2, \ldots, x_n$ be elements of $(\mathbb{T}, \oplus, \odot)$. Then one can define both monomials and polynomials in these variables on the tropical algebra. A *tropical polynomial* p in n variables is defined as the function $p\colon \mathbb{R}^n \to \mathbb{R}$,

$$p(x_1, \ldots, x_n) = a \odot x_1^{i_1} x_2^{i_2} \cdots x_n^{i_n} \oplus b \odot x_1^{j_1} x_2^{j_2} \cdots x_n^{j_n} \oplus \cdots\ , \tag{6}$$

with $a, b, \ldots \in \mathbb{R}$, $i_1, j_1, \ldots \in \mathbb{Z}$. According to the definition of tropical addition and multiplication we also have

$$p(x_1, \ldots, x_n) = \min(a + i_1 x_1 + \cdots + i_n x_n, b + j_1 x_1 + \cdots + j_n x_n, \ldots).$$

The following Lemma 1 tell us that a graph of tropical polynomial is consisted by linear functions.

Lemma 1 *Tropical polynomials in n variables $x_1, \ldots, x_n$ are linear piecewise concave functions on $\mathbb{R}^n$ with integer coefficients.*

The values of arguments of tropical polynomial function p in the breakpoints where p fails to be linear are zeros of p, the so-called hypersurface $V(p)$. As a concrete example of a tropical polynomial in one variable we consider

$$\begin{aligned} p(x) &= 3 \odot x^3 \oplus 1 \odot x^2 \oplus 2 \odot x \oplus 4 \\ &= \min(3 + 3x, 1 + 2x, 2 + x, 4). \end{aligned}$$

The graph of this function consists of four lines: $y = 3x + 3$, $y = 2x + 1$, $y = x + 2$ and $y = 4$ (see Figure 1) and related hypersurface is $V(p) = \{-2, 1, 2\}$. The fundamental theorem of algebra holds true also in tropical algebra, thus tropical polynomial function can be whiten as a tropical product of linear functions. In this particular example zeros are $-2, 1, 2$ so we have

$$p(x) = 3 \odot (x \oplus (-2)) \odot (x \oplus 1) \odot (x \oplus 2).$$

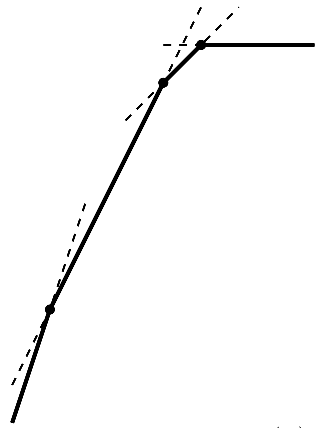


Figure 1: Graph of the tropical polynomial $p(x) = 3x^3 \oplus 1x^2 \oplus 2x \oplus 4$.

1.2 Shortest path, tropical distance and volume

We let G denote a directed graph with n nodes that are labeled by $1, 2, \ldots, n$. Every directed edge (i, j) in G has an associated length $d_{ij} \in \mathbb{R}_{\geq 0}$. If (i, j) is not an edge of G then we set $d_{i,j} = +\infty$. We represent the weighted directed graph G by its $n \times n$ adjacency matrix D_G,

$$D_G = \begin{pmatrix} 0 & d_{1,2} & \cdots & d_{1,n} \\ d_{2,1} & 0 & \cdots & d_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ d_{n,1} & d_{n,2} & \cdots & 0 \end{pmatrix}.$$

Off-diagonal entries are the edge lengths d_{ij}. The matrix D_G need not be symmetric. Now, consider the $n \times n$ matrix which is obtained from topically multiplying the given adjacency matrix D_G with itself $n - 1$ times

$$D_G^{\odot n-1} = D_G \odot D_G \odot \cdots \odot D_G.$$

The problem of finding shortest paths in a weighted directed graph G is solved in the following Lemma 2.

Lemma 2 *Let G be a weighted directed graph on n nodes with $n \times n$ adjacency matrix D_G. The entry of the matrix $D_G^{\odot n-1}$ in row i and column j equals the length of a shortest path from node i to node j in G.*

For $r \geq 0$, a recursive formula for the length of a shortest path from node i to node j which uses at most r edges in G we can write in the following way:

$$d_{ij}^{(r)} = \min\{d_{ik}^{(r-1)} + d_{kj} : k = 1, 2, \ldots, n\}.$$

This recursion is used in the *Floyd-Warshall algorithm*. This algorithm is known as the fastest algorithm for finding shortest paths in a weighted graph. For us, running that algorithm means performing the matrix multiplication

$$D_G^{\odot r} = D_G^{\odot r-1} \odot D_G \quad \text{for} \quad r = 2, \ldots n-1.$$

In this section we will still define tropical distance and tropical volume. For more see [4, 5]. For two points $v, w \in \mathbb{T}^d$ the *tropical distance* is the number

$$\begin{aligned} \operatorname{tdist}(v, w) &:= \max\{(v_i - w_i) \mid i \in [d]\} - \min\{(v_i - w_i) \mid i \in [d]\} \\ &= \max_{i,j \in [d]} |v_i - w_i + w_j - v_j| \qquad . \end{aligned}$$

This number is given in [4, 5] and he is the Euclidean distance in the tropical setting.

Let $A = (a_{ij}) \in \mathbb{T}^{d \times d}$ be a square matrix. *Tropical volume* of A is given as the expression

$$\operatorname{tvol} A := \left| \bigoplus_{\sigma \in \mathrm{Sym(d)}} \sum a_{i,\sigma(i)} \quad - \bigoplus_{\tau \in (\mathrm{Sym(d)} - \sigma_{opt})} \sum a_{i,\tau(i)} \right|$$

where σ_{opt} is a permutation for which $\sum a_{i,\sigma_{opt}(i)}$ coincides with the tropical determinant of A. *Tropical determinant* is defined in the following way

$$\operatorname{tropdet}(A) := \bigoplus_{\sigma \in S_n} x_{1\sigma(1)} \odot x_{2\sigma(2)} \odot \cdots \odot x_{n\sigma(n)}.$$

1.3 Tropical curves in $\mathbb{T}^2$

In the introduction we consider a graph of a tropical polynomial in one variable and have seen that such a graph is a collection of linear concave functions. Naturally an extension of this notion within polynomials of any degree and any number of variables lead to *tropical curves*. For the purpose to have conceptually simpler definitions and examples here we restrict discussion to curves in $\mathbb{T}^2$ instead of $\mathbb{T}^n$. In order to define tropical curve, we must first define tropical hypersurface we mentioned in the introduction. *Tropical hypersurface* $V(p)$ of p is the set of all points $w \in \mathbb{T}^2$ at which this minimum is attained at least twice. Equivalently, a point $w \in \mathbb{T}^2$ lies in $V(p)$ if and only if p is not linear at w. *Plane tropical curve* is tropical hypersurface $V(p)$ of a polynomial in two variables

$$p(x,y) = \bigoplus_{(i,j)} c_{ij} \odot x^i \odot y^j.$$

A tropical line of a 2-variable polynomial p is a hypersurface $V(p)$ of the first degree p,

$$p(x,y) = a \odot x \oplus b \odot y \oplus c = \min(a+x, b+y, c),$$

with $a, b, c \in \mathbb{R}$. This tropical line consists of three semi-lines with source in $(c-a, c-b)$ where directions of lines are north, east and south-west i.e. they are defined by relations $x = c - a \leq y$, $y = c - b \leq x$ and $y = x$, respectively. Figure 2 a) depicts such a line. In the same fashion one can study tropical quadratic curves as well as the other higher order curves. In general, tropical curve defined by $p(x,y)$ is a *graph* having defined the weight function on the edges, and this function is defined by means of the polynomial degree and the coefficients [2].

As an even more illustrative example let us consider a quadratic curve, defined by the polynomial $p(x,y) = a \odot x^2 \oplus b \odot xy \oplus c \odot y^2 \oplus d \odot y \oplus e \oplus f \odot x$. To draw the related curve one have to take into account 15 constraints arising from the definition of polynomial, which give the curve having three segments and six semi-lines. The Figure 2 b) shows a tropical conic defined by

$$p(x,y) = 2 \odot x^2 \oplus xy \oplus 2 \odot y^2 \oplus x \oplus (-1) \odot y \oplus 3.$$

The following Lemma 3 summarizes the salient features of a plane tropical curve.

Lemma 3 *The curve $V(p)$ is a finite graph that is embedded in the plane $\mathbb{R}^2$. It has both bounded and unbounded edges, all edge slopes are rational, and this graph satisfies a balancing condition around each node.*

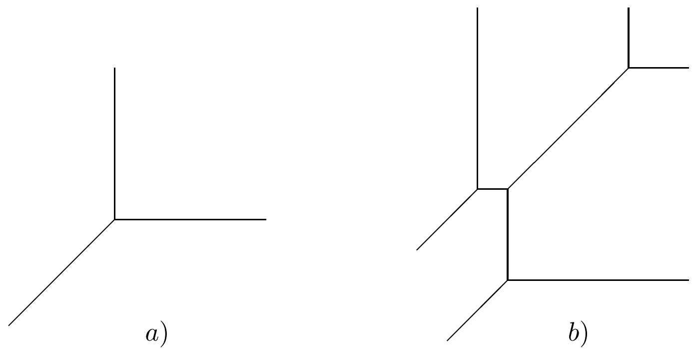


Figure 2: A tropical line and a tropical quadratic curve.

Below we give another way we can describe the tropical curves. The *Newton polygon* of the implicit equation $f(x, y)$ is the convex hull in $\mathbb{R}^2$ of all points $(i, j) \in \mathbb{Z}^2$ such that $x^i y^j$ appears with non-zero coefficient in the expansion of $f(x, y)$.

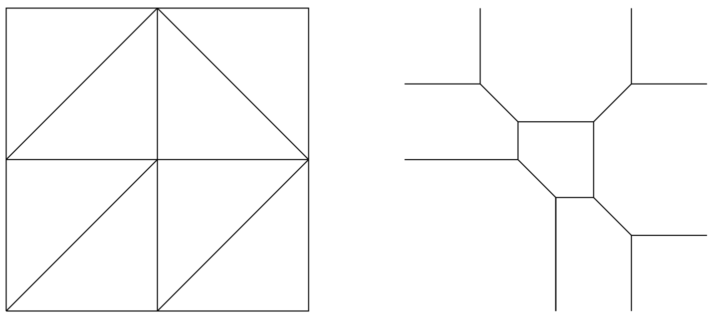
Lemma 4 *We let p is a tropical polynomial. Then $V(p)$ is a planar graph which is a dual of regular subdivision of the Newtonian polygon $Newt(p)$.*

The unbounded rays of a tropical curve $V(p)$ are perpendicular to the edges of the Newton polygon. The Figure 3 a) shows a subdivisions of the Newton polygon and the Figure 3 b) shows belongs to the tropical biquadratic curve.

Let consider tropical curves having Newtonian polygon being triangle with vertices $(0, 0)$, $(0, d)$ and $(d, 0)$. These curves we shall call *curves of the degree d*. The curve of the degree d has d semi-lines, taking into account multiplicity (the weights of edges), which are perpendicular to each of three edges of the Newtonian triangle [16, 22]. There are some facts known about intersection of two curves of a certain degree. We have it by the following Bézout's theorem (see [1, 9]).

Theorem 5 (Bézout) *We let C and D be two tropical curves of the degrees c and d in $\mathbb{R}^2$. If these curves intersect transversely then the number of intersecting points, counted with multiplicity, is equal to cd.*

On the other hand, it is possible that the two curves have no neither transversal nor finite intersection. This possibility is called *stable intersection* and more details on it one can find at [16].



a) b)

Figure 3: Subdivisions of a Newton polygon and the tropical biquadratic curve

1.4 Gromov-Witten invariants

A *complex algebraic curve* is the set of zeros of a homogeneous polynomial $P(x, y, z) = 0$ in the complex projective space $\mathbb{P}^2$. The degree of a complex algebraic curve is simply the degree of the polynomial $P(x, y, z)$ [7].

The central subject of the enumerative geometry is to determine Gromov-Witten invariants. This invariant counts how many of complex algebraic curves of a given degree and genus are incident with certain number of points. It is proven by G. Mikhalkin that complex algebraic curves can be replaced by tropical curves in that sense and he used this fact to derive combinatorial expression for the number of curves in the tropical case [8, 12, 13, 16].

Recall that if C is a smooth curve of the degree d in the projective plane $\mathbb{P}^2$, then its genus $g(C)$ is equal to

$$g(C) = \frac{1}{2}(d-1)(d-2).$$

We also have

$$g(C) = \#(\mathrm{int}(\mathrm{Newt}(C)) \cap \mathbb{Z}^3).$$

The set of all curves of the degree d forms projective space of the dimension

$$\binom{d+2}{2} - 1 = \frac{1}{2}(d-1)(d-2) + 3d - 1.$$

We let C_{sing} denote a singular curves having ν knots. Then for its genus we have $g(C_{\text{sing}}) = \frac{1}{2}(d-1)(d-2) - \nu$.

Now, the question arising is what is the number $N_{g,d}$ of irreducible curves of genus g and degree d, which are incident with $g + 3d - 1$ general points in a complex projective plane $\mathbb{P}^2$. It is remarkable fact that the number $N_{g,d}$ can be found and it can be done by methods of tropical geometry. In particular we have the following theorem, known as the Mikhailkin theorem of correspondence.

Theorem 6 *The number of irreducible tropical curves of the degree d and genus g which are incident with $g + 3d - 1$ general points in $\mathbb{R}^2$, where each curve is counted with multiplicity, is equal to the Gromov-Witten number $N_{g,d}$ of the complex projective plane $\mathbb{P}^2$.*

In order to illustrate this statement let us list several values of the Gromov-Witten invariants. The simplest Gromov-Witten invariants are $N_{0,1} = 1$ and $N_{0,2} = 1$. It state that a unique line passes through two points, and that a unique quadric passes through five points. The first non-trivial number is $N_{0,3} = 12$. We will explain it briefly. Let curves be defined as cubic polynomials

$$f = c_0x^3 + c_1x^2y + c_2x^2z + c_3xy^2 + c_4xyz + c_5xz^2 + c_6y^3 + c_7y^2z + c_8yz^2 + c_9z^3.$$

For general coefficients $c_0, c_1, \ldots, c_9$, the curve $\{f = 0\}$ is smooth of genus $g = 1$. The curve becomes rational, i.e. the genus drops to $g = 0$, precisely when it has a singular point. This is happening if and only if the discriminant of f vanishes. The discriminant $\Delta(f)$ is a homogeneous polynomial of degree 12 in the 10 coefficients $c_0, c_1, \ldots c_9$ which are unknown. It is a sum of 2040 monomials:

$$\Delta(f) = 19683c_0^4c_6^4c_9^4 - 26244c_0^4c_6^3c_7c_8c_9^3 + \cdots - c_2^2c_3c_4^4c_5^3c_6^2. \tag{7}$$

Discriminants (7) is calculated using [11]. Further, suppose the cubic $\{f = 0\}$ is required to pass through eight given points in $\mathbb{P}^2$. This translates into eight linear equations in $c_0, c_1, \ldots c_9$. Combining the equation $\Delta(f) = 0$ with the eight linear equations, we obtain a system of equations that has 12 solutions in $\mathbb{P}^9$. These solutions are the coefficient of the $N_{0,3} = 12$ rational cubics we seek.

The other non-trivial numbers are $N_{3,4} = 1$, $N_{2,4} = 27$, $N_{1,4} = 255$, $N_{0,4} = 620$. When $g = 0$ these values satisfy a nice recurrence relation

$$N_{0,d} = \sum_{\substack{d_1+d_2=d \\ d_1,d_2>0}} \left(d_1^2d_2^2 \binom{3d-4}{3d_1-2} - d_1^3d_2 \binom{3d-4}{3d_1-1} \right) N_{0,d_1}N_{0,d_2}. \tag{8}$$

1.5 Concluding remarks

Tropical geometry is a rather new field at the interface between algebraic geometry and combinatorics, and with connections to many other fields. Respectively it is a linear version of algebraic geometry in which polynomials are replaced with piecewise-linear functions, and their zero sets into polyhedral complexes. As such, it is suitable to study using the aid of combinatorics. It has shown that many algebraically difficult operations become easier in the tropical setting, as the structure of the objects seems to be simpler. Because of that tropical geometry has found significant applications, in particular in dynamic programming. In enumerative geometry many open problems are solved using ideas of tropical geometry. It also takes a role in physics, since it appears in the study of the string theory.

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On some partition identities related to affine Lie algebra representations

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Abstract

In this paper, meant for combinatorialists, we give a proof of equipotence of two families of partitions ('Primc conjecture') which appeared in the early stage of representation theory of affine Lie algebra $A_1^{(1)}$ (or $Sl(2,\mathbb{C})^\wedge$). The result was obtained already in 1983 and it lead to the very first character formulas for the level 3 standard modules (this is mentioned in Ref[1]) on pages 2 and 77 respectively). We hope that the intricacy of handling the interlocking recursion relations may be of some interest to combinatorialists not working in Lie algebra theory.

Keywords: partition function, partition identity, Lie algebra

MSC: 05A17, 11P84

1.1 Introduction

For $\nu = 0, 1, 2 \pmod 3$ we introduce the following families of partitions:

$$\begin{aligned} Q_s^\nu(n) := \{(n_0, n_1, ..., n_s) \in \mathbb{N}^{s+1} | & n = n_0 + n_1 + ... + n_s, \\ & n_i \equiv -i - \nu \pmod 3, \\ & n_i \geq n_{i+1} - 2,\ \ n_i > n_{i+2}\} \end{aligned} \tag{9}$$

$$Q^\nu(n) := \bigcup_{s \geq 0} Q_s^\nu(n)$$

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and denote by

$$q_s^\nu(n) := \mathrm{Card} Q_s^\nu(n) \tag{10}$$
$$q^\nu(n) := \mathrm{Card} Q^\nu(n) \tag{11}$$

the numbers of partitions in these families of partitions.

The partitions from (9) we shall relate to the partitions appearing in the Gordon's generalization of the Rogers-Ramanujan identities:

$$\begin{aligned} P_{k,i}(n,m) := \{(n_1,...,n_m) \in \mathbb{N}^m | n = n_1 + ... + n_m, \\ n_j \geq n_{j+1}, n_j \geq n_{j+k-1} + 2, \\ \mathrm{Card}\{j | n_j = 1 < i\}\} \end{aligned} \tag{12}$$

$$p_{k,i}(n,m) := \mathrm{Card} P_{k,i}(n,m) \tag{13}$$

Proposition 1 *The family $Q_s^\nu(n)$ is nonempty if $s \pmod 3$ is given by the following table,*

$n \pmod 3 \setminus \nu$	0	1	2
0	0 *or* 2	1 *or* 2	2
1	–	–	0 *or* 1
2	1	0	–

(14)

Proof. *For any given n, ν if $\alpha = (n_0,...,n_s) \in Q_s^\nu(n) \neq \emptyset$, then*

$$n \equiv \sum_{i=0}^{s}(-i-\nu) \pmod 3 = -\frac{s(s+1)}{2} - (s+1)\nu \pmod 3. \tag{15}$$

■

The recursions for the number theoretic functions $q_s^\nu(n)$ (defined by (23)) are given by the following proposition.

Proposition 2 *For $n \in \mathbb{N}$, $s \in \mathbb{Z}_+$, $\nu \in \mathbb{Z}_3$ we have:*

$$q_s^\nu(n) = \begin{cases} q_s^{\nu+2}(n-2s+2) + q_{s-2}^{\nu+2}(n-2s-2), & \textit{if } s+\nu \equiv 0 \pmod 3 \\ q_s^{\nu+1}(n-s-1), & \textit{if } s+\nu \equiv 1 \pmod 3 \\ q_s^{\nu+1}(n-s-1) + q_{s-1}^{\nu+2}(n-s-1), & \textit{if } s+\nu \equiv 2 \pmod 3 \end{cases} \tag{16}$$

with initial conditions

$$q_s^\nu(1) = \delta_{s,2} \cdot \delta_{s,0} \tag{17}$$

together with the convention $q_s^\nu(0) = 1$ *if* $s = \nu = 0$ *or* $s = -1, \nu = 1$*; 0 otherwise. We put*

$$q_s^\nu(n) = 0 \tag{18}$$

if $(s \leq 0$ *or* $n \leq 0)$ *and* $n \neq s$*, so that the right-hand side of (16) is well defined. With the recursions above all functions* $q_s^\nu(n)$ *are uniquely defined.*

Proof. *We distinguish three cases depending on* $(s+\nu) \pmod 3$*.* $s+\nu \equiv 0 (mod 3)$*. If* $s = 0$*, then* $\alpha = (n_0), n_0 \equiv -\nu (mod 3), n_0 > 0$*; so*

$$q_0^\nu(n) = \begin{cases} q_0^2(n-2), & \text{for } \nu = 0 \\ q_0^2(n-1), & \text{for } \nu = 1 \\ q_0^0(n-1), & \text{for } \nu = 2 \end{cases}.$$

If $s > 0$ *and* $\alpha = (n_0, ..., n_s) \in Q_s^\nu(n)$*, then* $n_{s-1} \equiv -(s-1) - \nu \equiv 1 (mod 3)$*,* $n_s = -s - \nu \equiv 0 (mod 3)$*, hence* $n_{s-1} \geq 1$*,* $n_s \geq 3$*. Then in the subcase a1)* $n_{s-1} \geq 2$ *we have* $n_{s-1} \geq 4$ *because* $n_{s-1} \equiv 1 (mod 3)$*. By letting* $\hat{\alpha} := (n_0 - 2, ..., n_s - 2)$ *we get all partitions from* $Q_s^{\nu+2}(n - 2s - 2)$*.*

In the subcase a 2) $n_{s-1} = 1$*, from (9) it follows* $n_{s-1} \geq n_s - 2$*, hence* $n_s = 3$*. So* $Q_1^2(4) = \{(1,3)\}$ *and* $q_1^2(4) = 1$*, and for* $s \geq 2$ *by letting*

$$\hat{\alpha} = (n_0 - 2, ..., n_{s-2} - 2)$$

we obtain all partitions from $Q_{s-2}^{\nu+2}(n - 2s - 2$*, because* $n_{s-2} > n_s (= 3)$*,* $n_{s-3} \geq n_{s-2} - 2 (\geq 1)$*.*

By combining the two bijections from a1) and a2) we obtain the first relation in (16).

b) $s + \nu \equiv 1 \pmod 3$*. For* $\alpha = (n_0, ..., n_s) \in Q_s^\nu(n)$*,* $n_s \equiv -s - \nu \equiv 2 \pmod 3$*,* $n_{s-1} \equiv -s + 1 - \nu \equiv 0 \pmod 3$*.*

So $n_s \geq 2$ *and* $n_{s-1} \geq 3$ *(if* $s > 0$*). Then the map* $\alpha \mapsto \bar{\alpha} = (n_0 - 1, ..., n_s - 1)$ *is a bijection onto* $Q_s^{\nu+1}(n - s - 1)$*.*

c) $s + \nu \equiv 2 \pmod 3$*. For* $\alpha = (n_0, ..., n_s) \in Q_s^\nu(n)$ *we have* $n_s \equiv 1 \pmod 3$ *and* $n_{s-1} \equiv 2 \pmod 3$ *(if* $s > 0$*). Like in a) we have two subspaces:*

c1) $n_s = 1$*. Then* $\alpha \mapsto \bar{\alpha} = (n_0 - 1, ..., n_{s-1} - 1)$ *is a bijection onto* $Q_{s-1}^{\nu+1}(n - s - 1)$*.*

c2) $n_s \geq 4$. *Then* $n_{s-1} \geq n_s - 2(\geq 2)$, *so we get a bijection* $\alpha \mapsto \bar{\alpha} = (n_0-1, ..., n_s-1)$ *onto* $Q_s^{\nu+1}(n-s-1)$. *In the case* $s=0$, *we have* $\nu \equiv 2 \pmod 3$ *we need to check that* $q_0^2(n) = q_0^0(n-1)$. *For* $n > 1$ *it is obvious, and for* $n=1$, $q_0^{(2)}(1) = 1 = q_0^0(0)$ *by (18).*

The fact that (16) uniquely determines the functions q_s^ν *one can prove by induction on* $n+s$. ■

Corollary 3 *For* $n \in \mathbb{N}, s \in \mathbb{Z}_+, \nu \in \mathbb{Z}_3$ *(with the conventions from the Proposition 2) we have*

$$\begin{aligned} q_{s+2}^\nu(n) + q_s^\nu(n) &= q_{s+2}^{\nu+1}(n+2s+6), \quad \text{if } s+\nu \equiv 0 \pmod 3 \\ q_s^\nu(n) &= q_s^{\nu+2}(n+s+1), \quad \text{if } s+\nu \equiv 2 \pmod 3 \\ q_{s+1}^\nu(n) + q_s^\nu(n) &= q_{s+1}^{\nu+2}(n+s+2), \quad \text{if } s+\nu \equiv 2 \pmod 3 \end{aligned} \tag{19}$$

Corollary 4 *For the number theoretic functions* $q^\nu(n)$, $(\nu = 0,1,2)$ *defined in (11) we have the following formulas:*

$$
\begin{array}{ll}
i) & q^0(3n) = \sum_{s\geq 1} q^1_{3s-1}(3n+6s) \\
ii) & q^0(3n) = \sum_{s\geq 0} q^2_{3s}(3n+3s+1) = \sum_{s\geq 0} q^0_{3s}(3n+6s+2) \\
iii) & q^1(3n) = \sum_{s\geq 1} q^2_{3s-1}(3n+6s+4) \\
iv) & q^1(3n) = \sum_{s\geq 1} q^0_{3s-1}(3n+3s) \\
v) & q^2(3n+1) = \sum_{s\geq 1} q^1_{3s-2}(3n+3s) = \sum_{s\geq 1} q^0_{3s-2}(3n+6s-1) \\
vi) & q^2(3n+1) = \sum_{s\geq 0} q^0_{3s}(3n+6s+3) \\
vii) & q^2(3n) = \sum_{s\geq 0} q^2_{3s+2}(3n) = \sum_{s\geq 1} q^0_{3s-1}(3n-3s) \\
viii) & q^0(3n+2) = \sum_{s\geq 0} q^0_{3s+1}(3n+2) = \sum_{s\geq 0} q^1_{3s+1}(3n-3s) \\
ix) & q^1(3n+2) = \sum_{s\geq 0} q^1_{3s}(3n+2) = \sum_{s\geq 0} q^2_{3s}(3n-3s+1) \\
x) & q^0(3n+1) = q^1(3n+1) = q^2(3n+2) = 0.
\end{array}
\tag{20}
$$

Proof. *Follows easily by Corollary 3 with the help of Proposition 1.* ■

1.2 Relation to Gordon partitions

In this subsection we shall relate partition families $Q^\nu_s(n)$ from (9) firstly to standard partitions with additional difference conditions and secondly to Gordon partitions. For $n \in \mathbb{N}$, $s \in \mathbb{Z}_+$, $\nu \in \mathbb{Z}_3$ we introduce the following families of partitions:

$$
\begin{aligned}
\bar{Q}^\nu_s(n) &:= \{(n_0, n_1, ..., n_s) \in \mathbb{N}^{s+1} | n_j \equiv -s-\nu (mod 3), \\
&\qquad n = n_0 + ... + n_s, n_j \geq n_{j+1}, n_j - n_{j+2} \geq 5, n_{s-1} > 2\} \\
\bar{Q}^\nu(n) &:= \bigcup_{s\geq 0} \bar{Q}^\nu_s(n)
\end{aligned}
\tag{21}
$$

and denote by

$$\bar{q}_s^{\nu}(n) := \mathrm{Card}\bar{Q}_s^{\nu}(n) \tag{22}$$
$$\bar{q}^{\nu}(n) := \mathrm{Card}\bar{Q}^{\nu}(n). \tag{23}$$

Proposition 3 *For any $n \in \mathbb{N}$ and $0 \leq s \leq n$ we have*

$$q_s^{\nu}(n) = \bar{q}_s^{\nu}(n + s(s+1)) \tag{24}$$

Proof. *For $\alpha = (n_0, ..., n_s) \in Q_s^{\nu}(n)$ let $\alpha' = (n_0^{'}, ..., s_s^{'})$ be defined by*

$$n_i^{'} = n_i + 2(s-i).$$

We claim that $\alpha \mapsto \alpha^{'}$ is a bijection of $Q_s^{\nu}(n)$ with $\bar{Q}_s^{\nu}(n)$. From $\sum_{i=0}^{s} 2(s-i) = s(s+1)$ and $n_i^{'} = n_i + 2(s-i) \geq n_{i+1} - 2 + 2(s-i) = n_{i+1}^{'}$ it follows that $\alpha^{'}$ is a partition of $n + s(s+1)$. Since $n_i^{'} \equiv -i - \nu + 2(s-i) \equiv -s - \nu \pmod 3)$,

$$n_i^{'} = n_i + 2(s-i) > n_{i+2} + 2(s-i) = n_{i+2}^{'} + 4$$

and

$$n_{s-1}^{'} = n_{s-1} + 2 > 2.$$

then the partition $\alpha^{'}$ belongs to $\bar{Q}_s^{\nu}(n + s(s+1))$.

Conversely for any partition $\beta = (m_0, m_1, ..., m_s) \in \bar{Q}_s^{\nu}(n + s(s+1))$ let $\alpha = (n_0, ..., n_s)$, where $n_i := m_i - 2(s-i)$. Then $n_i \in \mathbb{N}$, because for $i = s - 2j$

$$n_{s-2j} = m_{s-2j} - 4j > m_{s-2j+2} - 4(j-1) > ... > m_s > 0$$

and for $i = s - 2j - 1$

$$n_{s-2j-1} = m_{s-2j-1} - 4j - 2 > ... > m_{s-1} - 2 > 0$$

where we have used the defining inequalities in $\bar{Q}_s^{\nu}(n)$ twice. Thus we have proved that $\alpha \mapsto \alpha^{'}$ is a bijection, hence the identity (24) follows. ■

Now we shall relate the partition families $\bar{Q}_s^{\nu}(n)$ to the Gordon's partitions families defined in (12).

Proposition 4 *In terms of the numbers $p_{k,i}(n,m)$ of Gordon partitions defined in (12) we have the following formulas:*

$$\bar{q}_s^{\nu}(n) = \begin{cases} p_{3,3}(\frac{n}{3}, s+1), & \text{if } s+\nu \equiv 0 \pmod 3, n \equiv 0 \pmod 3 \\ p_{3,2}(\frac{n+s+1}{3}, s+1), & \text{if } s+\nu \equiv 1 \pmod 3, n \equiv 2s+2 \pmod 3 \\ p_{3,2}(\frac{n+2s+2}{3}, s+1), & \text{if } s+\nu \equiv 2 \pmod 3, n \equiv s+1 \pmod 3 \end{cases}$$

Proof. *1.) Let $s+\nu \equiv 0 \pmod 3$. Then each $\alpha = (n_0, n_1, ..., n_s) \in \bar{Q}_s^{\nu}(n)$ satisfies $n_i \equiv 0 \pmod 3$, $n_i \geq n_{i+1}$, $n_i - n_{i+2} \geq 5$, $n_{s-1} > 2$. By defining $\alpha' = (m_0, ..., m_s)$, with $m_i = n_i/3$ we see that $m_i \geq m_{i+1}$, $m_i \in \mathbb{N}$, $m_i - m_{i+2} \geq 2$, $m_{s-1} > 1$. This implies that $\alpha' \in P_{3,3}(\frac{n}{3}, s+1)$ and clearly $\alpha \mapsto \alpha'$ is a bijection.*

2.) $s+\nu \equiv 1 \pmod 3$. Then $n_i \equiv 2 \pmod 3$, $n_i \geq n_{i+1}$, $n_i - n_{i+2} \geq 5$, $n_{s-1} > 2 (\implies n_{s-1} \geq 5)$. By defining $\alpha' = (m_0, ..., m_s)$ where $m_i = (n_i+1)/3$ we see that $m_i \geq m_{i+1}$, $m_i - m_{i+2} \geq 2$, $m_{s-1} > 1$ so α' belongs to $P_{3,2}(\frac{n+s+1}{3}, s+1)$ and again $\alpha \mapsto \alpha'$ is a bijection.

3.) $s+\nu \equiv 2 \pmod 3$. Then $n_i \equiv 1 \pmod 3$, $n_{s-1} > 2 (\implies n_{s-1} \geq 4)$. Let $\alpha' = (m_0, ..., m_s)$ where $m_i = (n_i+2)/3$. Then $m_i \in \mathbb{N}$, $m_i - m_{i+2} \geq 2$, $m_{s-1} > 1$. So $\alpha' \in P_{3,2}(\frac{n+2s+2}{3}, s+1)$ and $\alpha \mapsto \alpha'$ is a bijection. The proof is finished. ■

By combining the Proposition 3 and Proposition 4 we obtain

Corollary 5 *For any $n \in \mathbb{N}$ and $0 \leq s \leq n$, $\nu \in \{0,1,2\}$ we have*

$$q_s^{\nu}(n) = \begin{cases} p_{3,3}(\frac{n+s(s+1)}{3}, s+1), & \text{if } s+\nu \equiv 0 \pmod 3 \\ p_{3,2}(\frac{n+(s+1)^2}{3}, s+1), & \text{if } s+\nu \equiv 1 \pmod 3 \\ p_{3,2}(\frac{n+(s+1)(s+2)}{3}, s+1), & \text{if } s+\nu \equiv 2 \pmod 3 \end{cases}$$

where $p_{3,i}(n,m)$ is the number of partitions $(n_1, ..., n_m)$ of $n (= n_1 + ... + n_m)$ such that $n_j - n_{j+2} \geq 2$, $Card\{j | n_j = 1\} < i$. (cf. (12))

Remark 5 *We have*

i) $p_{3,3}(n,m) \neq 0 \implies m^2 \leq 2n$

ii) $p_{3,2}(n,m) \neq 0 \implies m(m+1) \leq 2n$

For i), if $(n_1, ..., n_m) \in P_{3,3}(n, m)$ *then*

$$n = n_1 + ... + n_m \geq \begin{cases} (m + (m-1) + (m-1) + ... + 3 + 3 + 1 + 1 = \frac{m^2+1}{2}, & \text{if } m \text{ odd} \\ ((m-1) + (m-1) + ... + 3 + 3 + 1 + 1 = \frac{m^2}{2}, & \text{if } m \text{ even} \end{cases}$$

For ii), if $(n_1, ..., n_m) \in P_{3,2}(n, m)$ *then*

$$n = n_1 + ... + n_m \geq m + (m-1) + ... + 2 + 1 = m(m+1)/2.$$

Remark 6 *We have*

$$q_s^\nu(n) \neq 0 \implies \begin{cases} (s+2)^2 < 2n, & \text{if } s + \nu \equiv 0 \pmod 3 \\ (s+1)(s+4) \leq 2n, & \text{if } s + \nu \equiv 1 \pmod 3 \\ (s+1)(s+2) \leq 2n, & \text{if } s + \nu \equiv 2 \pmod 3. \end{cases}$$

1.3 Equipotence of the families $Q^\nu(n), \nu = 0, 1$ of partitions

Theorem 7 *For* $n \in 3\mathbb{N}$, $\nu = 0, 1$, *the set of partitions*

$$\begin{aligned} Q^\nu(n) := \{(n_0, n_1, ..., n_s) \in \mathbb{N}^{s+1} \quad | \quad & n_i \equiv -i - \nu \pmod 3, s \geq 0, \\ & n = n_0 + ... + n_s, \\ & n_i > n_{i+2}, \\ & n_i \geq n_{i+1} - 2\} \end{aligned}$$

are equinumerous, i.e. Card $Q^0(n) =$ *Card* $Q^1(n)$.

Proof. We have to prove that Card$Q^0(n)$ = Card$Q^1(n)$ ($n \in 3\mathbb{N}$) or, by using the notation (11) that

$$q^0(n) = q^1(n), \;\; n \in 3\mathbb{N} \tag{25}$$

By relations (20) i), iv) of Corollary 4 this is equivalent to

$$\sum_{s \equiv 2 \pmod 3} q_s^1(n + 2s + 2) = \sum_{s \equiv 2 \pmod 3} q_s^0(n + s + 1), \;\; n \in 3\mathbb{N}, \;\; s \geq 0 \tag{26}$$

and, by Corollary 5. this is equivalent to

$$\sum_{s\equiv 0 \pmod 3} p_{3,3}\left(\frac{n+s(s+1)}{3}, s\right) = \sum_{s\equiv \pmod 3} p_{3,2}(\frac{n+s(s+2)}{3}, s), \tag{27}$$

with $n \in 3\mathbb{N},\ \ s > 0.$

Now we employ the Theorem 1 of reference [2] in the special case $k = 3, i = 2, 3, d = 0$. In our notations (13) and by replacing q for q^3 special case reads as follows:

$$\sum_{n\geq 0}\sum_{m\geq 0} p_{3,i}(n,m)q^{3n}z^m = \sum_{n_1\geq 0}\sum_{n_2\geq 0} \frac{z^{N_1+N_2}}{(q^3)_{n_1}(q^3)_{n_2}} \begin{cases} q^{3(N_1^2+N_2^2)}, & \text{if } i=3 \\ q^{3(N_1^2+N_2^2+N_2)}, & \text{if } i=2 \end{cases} \tag{28}$$

where $N_1 = n_1 + n_2,\ N_2 = n_2$ and $(q)_k = (1-q)(1-q^2)...(1-q^k)$. From (28) it follows easily

$$\begin{aligned} p_{3,3}\left(\frac{n+s(s+1)}{3}, s\right) &= [q^{n+s(s+1)}] \sum_{n_1,n_2\geq 0, N_1+N_2=s} \frac{q^{3(N_1^2+N_2^2)}}{(q^3)_{n_1}(q^3)_{n_2}} \\ &= [q^n] \sum_{n_1,n_2\geq 0, N_1+N_2=s} \frac{q^{3N_1^2+3N_2^2-s(s+1)}}{(q^3)_{n_1}(q^3)_{n_2}} \\ &= [q^n] \sum_{n_1,n_2\geq 0, N_1+N_2=s} \frac{q^{2(N_1^2-N_1N_2+N_2^2)-N_1-N_2}}{(q^3)_{n_1}(q^3)_{n_2}}. \end{aligned} \tag{29}$$

Similarly we get

$$p_{3,2}\left(\frac{n+s(s+2)}{3}, s\right) = [q^n] \sum_{n_1,n_2\geq 0, N_1+N_2=s} \frac{q^{2(N_1^2-N_1N_2+N_2^2)+N_2-2N_1}}{(q^3)_{n_1}(q^3)_{n_2}}. \tag{30}$$

From (25) $\Longleftrightarrow$ (26) $\Longleftrightarrow$ (27) and (29) , (30) to prove (25) it is enough to prove the equality of generating functions

$$1+\sum_{n\geq 1, n\equiv 0 \pmod 3} q^0(n)x^n = \sum_{n_1,n_2\geq 0, N_1+N_2\equiv 0 \pmod 3} \frac{x^{2(N_1^2-N_1N_2+N_2^2)-N_1-N_2}}{(x^3)_{n_1}(x^3)_{n_2}} \tag{31}$$

and

$$1+\sum_{n\geq 1, n\equiv 0 \pmod 3} q^1(n)x^n = \sum_{n_1,n_2\geq 0, N_1+N_2\equiv 0 \pmod 3} \frac{x^{2(N_1^2-N_1N_2+N_2^2)+N_2-2N_1}}{(x^3)_{n_1}(x^3)_{n_2}} \tag{32}$$

Observe now that for $(n_1, n_2 \in \mathbb{N}^2)$ we have

$$n_1 + 2n_2 \equiv 0 \pmod 3 \Longleftrightarrow n_2 + 2n_1 \equiv 0 \pmod 3.$$

By change of variables $(n_1, n_2) \to (n_2, n_1)$ in (32), the quantity $N_2 - 2N_1 = n_2 - 2(n_1 + n_2) = -2n_1 - n_2$ gets transformed to $-n_1 - 2n_2 = -N_1 - N_2$ and the R.H.S of (32) becomes the R.H.S of (31) so the R.H.S of (31) and (32) are equal. This proves the Theorem 7

■

Theorem 8 *For the functions $q^{(0)}(n)$, $q^{(1)}(n)$, $q(n)$ we have the following generating functions:*

$$i)\ 1+\sum_{n\equiv 0 \pmod 3} q^{(0)}(n)x^n = \sum_{n_1,n_2\geq 0, N_1+N_2\equiv 0 \pmod 3} \frac{x^{2(N_1^2-N_1N_2+N_2^2)-N_1-N_2}}{(x^3)_{n_1}(x^3)_{n_2}} \tag{33}$$

$$ii)\ \sum_{n\equiv 0 \pmod 3} q^{(1)}(n)x^n = \sum_{n_1,n_2\geq 0, N_1+N_2\equiv 2 \pmod 3} \frac{x^{2(N_1^2-N_1N_2+N_2^2)-N_1-N_2}}{(x^3)_{n_1}(x^3)_{n_2}} \tag{34}$$

$$iii)\ \sum_{n\equiv 1 \pmod 3} q^{(2)}(n)x^n = \sum_{n_1,n_2\geq 0, N_1+N_2\equiv 1 \pmod 3} \frac{x^{2(N_1^2-N_1N_2+N_2^2)-N_1-N_2}}{(x^3)_{n_1}(x^3)_{n_2}} \tag{35}$$

Proof. The relation *i*) is obtained in (31). In order to prove relation *ii*) we use (20), *iii*) to get

$$q^{(1)}(n) = \sum_{s\in 3\mathbb{Z}_+ +1} q_s^{(2)}(n+2s+2).$$

Furthermore, according to Corollary 5 we have

$$\begin{aligned} q^{(1)}(n) &= \sum_{s\in 3\mathbb{Z}_+ +1} p_{3,3}\left(\frac{n+(s+1)(s+2)}{3}, s+1\right) \\ &= \sum_{t\in 3\mathbb{Z}_+ +2} [x^{n+t(t+1)}] \sum_{n_1,n_2\geq 0, N_1+N_2\equiv 2 \pmod 3} \frac{x^{(3N_1^2+3N_2^2)}}{(x^3)_{n_1}(x^3)_{n_2}} \\ &= [x^n] \sum_{n_1,n_2\geq 0, N_1+N_2\equiv 2 \pmod 3} \frac{x^{2(N_1^2-N_1N_2+N_2^2)-N_1-N_2}}{(x^3)_{n_1}(x^3)_{n_2}}. \end{aligned}$$

Now, by substitution into generating function for $q^{(1)}$ we obtain relation *ii*).

For the purpose to to prove relation *iii*) firstly we use relation *vi*) in Corollary 5 to get:

$$\begin{aligned} q^{(2)}(n) &= \sum_{s\in 3\mathbb{Z}_+ +1} q_s^{(0)}(n+2s+2), \;\; n\equiv 1 \pmod 3 \\ &= \sum_{s\in 3\mathbb{Z}_+} p_{3,3}\left(\frac{n+(s+1)(s+2)}{3}, s+1\right) \\ &= \sum_{t\in 3\mathbb{Z}_+ +1} [x^{n+t(t+1)}] \sum_{n_1,n_2\geq 0, N_1+N_2\equiv t \pmod 3} \frac{x^{(3N_1^2+3N_2^2)}}{(x^3)_{n_1}(x^3)_{n_2}} \\ &= [x^n] \sum_{n_1,n_2\geq 0, N_1+N_2\equiv 1 \pmod 3} \frac{x^{2(N_1^2-N_1N_2+N_2^2)-N_1-N_2}}{(x^3)_{n_1}(x^3)_{n_2}}. \end{aligned}$$

Once having this relation, the statement *iii*) follows directly. ■

Corollary 6 *We let χ denote the generating function which is the sum of generating function of i), ii) and iii) in Theorem 8. Then, we have*

$$\chi = \sum_{n_1,n_2\geq 0} \frac{x^{2(N_1^2-N_1N_2+N_2^2)-N_1-N_2}}{(x^3)_{n_1}(x^3)_{n_2}}. \tag{36}$$

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The Prouhet–Tarry–Escot Problem

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Abstract

An known elementary proof of existence of infinitely many solutions (and a procedure of their construction) to the Prouhet-Tarry-Escott problem is given together with its connection to the Prouhet–Thue–Morse sequence. Another very short and possibly not yet published proof is presented utilizing Taylor expansion of a suitably chosen function represented in two different ways.

The Prouhet-Tarry-Escott problem is a classical problem in Diophantine equations that consists of finding two different lists (i.e. multisets) of integers $[a_1, a_2, \dots a_n]$ and $[b_1, b_2, \dots b_n]$ (repetitions are allowed) such that

$$\begin{array}{ccccccccccc} a_1 & + & \cdots & + & a_n & = & b_1 & + & \cdots & + & b_n \\ a_1^2 & + & \cdots & + & a_n^2 & = & b_1^2 & + & \cdots & + & b_n^2 \\ \vdots & & & & & \vdots & & & & & \vdots \\ a_1^m & + & \cdots & + & a_n^m & = & b_1^m & + & \cdots & + & b_n^m \end{array}$$

where m and n are some natural numbers. It is known that n must be strictly greater than m (of special interest are so called ideal solutions where $m = n - 1$). The above system can be written as $[a_i] =_m [b_i]$. The earliest occurrence of a problem of this kind can be traced down to Euler and Goldbach 1750–1751 when they noted that

$$[a, b, c, a + b + c] =_2 [a + b, a + c, b + c].$$

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The problem was named after E. Prouhet, who studied it in the early 1850s, and G. Tarry and Escott, who studied it in the early 1910s.

We shall restrict the problem to disjoint sets (or multisets).

Definition 1 *Two finite sets (or multisets) $A, B \subset \mathbb{C}$ are said to have (or satisfy) n–property if $A, B \neq \emptyset$, $A \cap B = \emptyset$ and for any $k \in \{0, 1, 2, \ldots, n-1\}$ we have*

$$\sum A^k := \sum_{a\in A} a^k = \sum_{b\in B} b^k = \sum B^k.$$

Example 2 *The sets $A := \{0, 3, 5, 6\}$ and $B := \{1, 2, 4, 7\}$ have 3–property because*

$$\begin{aligned}
\sum A^0 &= 0^0 + 3^0 + 5^0 + 6^0 = \ \ 4 = 1^0 + 2^0 + 4^0 + 7^0 = \sum B^0 \\
\sum A^1 &= 0^1 + 3^1 + 5^1 + 6^1 = 14 = 1^1 + 2^1 + 4^1 + 7^1 = \sum B^1 \\
\sum A^2 &= 0^2 + 3^2 + 5^2 + 6^2 = 70 = 1^2 + 2^2 + 4^2 + 7^2 = \sum B^2.
\end{aligned}$$

Definition 3 *Let $S \subseteq \mathbb{C}$ and $c \in \mathbb{C}$. Then we define*

$$S + c := \{s + c \mid s \in S\}.$$

Lemma 4 *Let $A, B \subset \mathbb{C}$ satisfy n–property. Then for any $c \in \mathbb{C}$ the sets $A + c$ and $B + c$ also have n–property.*

Proof.

$$\begin{aligned}
\sum (A+c)^k &= \sum_{a\in A} (a+c)^k = \sum_{a\in A}\sum_{j=0}^{k} \binom{k}{j} a^j c^{k-j} = \sum_{j=0}^{k} \binom{k}{j} c^{k-j} \sum_{a\in A} a^j = \\
&= \sum_{j=0}^{k} \binom{k}{j} c^{k-j} \sum_{b\in B} b^j = \sum (B+c)^k \qquad \blacksquare
\end{aligned}$$

Example 5 *The sets $C = A - 4 = A + (-4) = \{-4, -1, 1, 2\}$ and $D = B - 4 = \{-3, -2, 0, 3\}$, where A and B are the same as in Example 2, also have 3–property:*

$$\begin{aligned}
\sum C^0 &= \ \ \ 4 = \sum D^0 \\
\sum C^1 &= -2 = \sum D^1 \\
\sum C^2 &= \ 22 = \sum D^2.
\end{aligned}$$

Lemma 6 *Let $A, B, C, D \subset \mathbb{C}$ and $(A \cup B) \cap (C \cup D) = \emptyset$. Then if two pairs of sets A, B and C, D both have n–property then the sets $A \cup C$ and $B \cup D$ also have n–property.*

Proof. Obvious. ∎

Proposition 7 *If sets $A, B \subset \mathbb{C}$ have n–property then for any $c \in \mathbb{C}$ such that $(A \cup B) \cap ((A+c) \cup (B+c)) = \emptyset$ sets $A_1 = (B+c) \cup A$ and $B_1 = (A+c) \cup B$ have $(n+1)$–property.*

Proof. Lemmas 4 and 6 imply that the sets A_1 and B_1 have n–property. It is easy to check that $A_1 \cap B_1 = \emptyset$. Now we have to prove that equality $\sum A_1^n = \sum B_1^n$ holds:

$$\begin{aligned}
\sum A_1^n &= \sum((B+c) \cup A)^n = \sum(B+c)^n + \sum A^n \\
&= \sum B^n + \sum_{j=0}^{n-1} \binom{n}{j} c^{n-j} \sum_{b \in B} b^j + \sum A^n \\
&= \sum B^n + \sum_{j=0}^{n-1} \binom{n}{j} c^{n-j} \sum_{a \in A} a^j + \sum A^n \\
&= \sum B^n + \sum(A+c)^n \\
&= \sum B_1^n. \qquad \blacksquare
\end{aligned}$$

Example 8 *Let A and B are as in Example 2. If we set $c = 8$ then $A_1 = \{0, 3, 5, 6, 9, 10, 12, 15\}$ and $B_1 = \{1, 2, 4, 7, 8, 11, 13, 14\}$ have 4–property:*

$$\begin{aligned}
\sum A_1^0 &= 8 = \sum B_1^0 \\
\sum A_1^1 &= 60 = \sum B_1^1 \\
\sum A_1^2 &= 620 = \sum B_1^2 \\
\sum A_1^3 &= 7200 = \sum B_1^3
\end{aligned}$$

Example 9 *Starting with $A_0 := \{0\}$ and $B_0 := \{i\}$ (note that any pair of singletons has 1–property) and taking $c_1 := 1$ and then $c_2 := \sqrt{2}$ we obtain (applying the procedure* *from Proposition 7 twice)* $A_2 = \{0, 1+i, i+\sqrt{2}, 1+\sqrt{2}\}$ *and* $B_2 = \{1, i, \sqrt{2}, 1+\sqrt{2}+i\}$ *that have* 3*–property:*

$$\begin{array}{rcl} \sum A_2^0 = & 4 & = \sum B_2^0 \\ \sum A_2^1 = & 2(1+\sqrt{2}+i) & = \sum B_2^1 \\ \sum A_2^2 = & 4+2\sqrt{2}+(2+2\sqrt{2})i & = \sum B_2^2 \end{array}$$

Example 10 *The sets* $A_0 := \{0\}$ *and* $B_0 := \{1\}$ *have* 1*–property. Suppose that sets* A_{n-1} *and* B_{n-1} *have* n*–property. Then by Proposition 7 for* $c_n := 1+\max(A_{n-1}\cup B_{n-1})$ *the sets* $A_n := A_{n-1}\cup(B_{n-1}+c_n)$ *and* $B_n := B_{n-1}\cup(A_{n-1}+c_n)$ *have* $(n+1)$*–property. By the definition of* c_n *it follows that* $\max(A_{n-1}\cup B_{n-1}) < c_n \le \min((A_{n-1}+c_n)\cup(B_n+c_n))$ *which proves that* $(A_{n-1}\cup B_{n-1})\cap((A_{n-1}+c)\cup(B_{n-1}+c)) = \emptyset$.

Lemma 11 *Let* $\alpha_2(m)$ *be the sum of digits of binary representation of number* m*. The sets* A_n *and* B_n *defined in Example 10 can be characterized in the following way:*

$$A_n = \{m \in \{0,1,2,\ldots,2^{n+1}-1\} \mid \alpha_2(m) \in 2\mathbb{N}\},$$
$$B_n = \{m \in \{0,1,2,\ldots,2^{n+1}-1\} \mid \alpha_2(m) \in 2\mathbb{N}+1\},$$

i.e., A_n *is the set of all natural numbers less than* 2^{n+1} *having even number of digits* 1 *in their binary representations. Likewise,* B_n *consists of all natural numbers less than* 2^{n+1} *having odd number of digits* 1 *in their binary representations. Note that* $c_n = 2^{n+1}$.

Proof. By induction on n we prove the statement of the Lemma 11 and that $c_n = 2^{n+1}$. Induction base is clear. Suppose now that

$$A_{n-1} = \{m \in \{0,1,2,\ldots,2^{n}-1\} \mid \alpha_2(m) \in 2\mathbb{N}\},$$
$$B_{n-1} = \{m \in \{0,1,2,\ldots,2^{n}-1\} \mid \alpha_2(m) \in 2\mathbb{N}+1\}.$$

and $c_n = 2^n$. By definition we have

$$A_n = A_{n-1}\cup(B_{n-1}+c_n),$$
$$B_n = B_{n-1}\cup(A_{n-1}+c_n).$$

Also, $\max(A_n\cup B_n) = c_n + \max(A_{n-1}\cup B_{n-1}) = 2c_n - 1 = 2^{n+2}-1$, so $c_{n+1} = 2^{n+2}$. Now, $(B_{n-1}+c_n) = \{m \in \{0,1,2,\ldots,2^n-1\} \mid \alpha_2(m) \in 2\mathbb{N}+1\} + 2^{n+1}$, so $A_n = A_{n-1}\cup(B_{n-1}+c_n) = \{m \in \{m \in \{0,1,2,\ldots,2^{n+1}-1\} \mid \alpha_2(m) \in 2\mathbb{N}\}$. (Adding $c_n = 2^n$ to numbers of B_{n-1} is equivalent to prefixing their binary representation with 1 together with some zeroes if necessary.) The proof for B_n is analogous.■

Remark 12 *The sequence* $t_n := \alpha_2(n) \bmod 2$ *is known as the Prouhet–Thue–Morse sequence (see [1] or [2], example 12.). Sets* A_n *and* B_n *can be characterized as follows:*

$$A_n = \{m \in \{0,1,2,\ldots,2^{n+1}-1\} \mid t_m = 0\},\ B_n = \{m \in \{0,1,2,\ldots,2^{n+1}-1\} \mid t_m = 1\}.$$

In other wording A_n (resp. B_n) consists of all nonnegative integers less than 2^{n+1} which are expressible as a sum of even (resp. odd) number of powers of 2.

Now we can elucidate this remarkable property by generalizing A_n (resp. B_n) to be sum of even (resp. odd) numbers of indeterminates $x_0, \ldots, x_{n-1}$. (Then Lemma 11 is just a very special case $x_k = 2^k$.)
The existence of different finite sets (of numbers) A and B having the n–property for any n can be proved quickly by using Taylor expansion of the following function $F := \prod_{j=0}^{n-1}(1-e^{tx_j})$. We have

$$\begin{aligned}
F &= \prod_{j=0}^{n-1}(1-e^{tx_j}) = \\
&= 1-(e^{tx_0}+\cdots+e^{tx_{n-1}})+\left(e^{t(x_0+x_1)}+\cdots+e^{t(x_{n-2}+x_{n-1})}\right)-\cdots = \\
&= \sum_{r=0}^{n}(-1)^r \sum_{0\le j_1<\cdots<j_r<n} e^{t(x_{j_1}+\cdots+x_{j_r})} = \\
&= \sum_{k=0}^{\infty}\sum_{r=0}^{n}\frac{(-1)^r}{k!}t^k \sum_{0\le j_1<\cdots<j_r<n}(x_{j_1}+\cdots+x_{j_r})^k\,.
\end{aligned}$$

On the other hand we have

$$\begin{aligned}
F &= \prod_{j=0}^{n-1}\left(-tx_j-\frac{t^2x_j^2}{2!}-\frac{t^3x_j^3}{3!}-\cdots\right) = \\
&= (-1)^n x_0x_1\cdots x_{n-1}t^n\prod_{j=0}^{n-1}\left(1+\frac{tx_j}{2!}+\frac{t^2x_j^2}{3!}+\cdots\right)\,.
\end{aligned}$$

Now for $k<n$ we get

$$0 = k![t^k]F = \sum_{r=0}^{n}(-1)^r\sum_{0\le j_1<\cdots<j_r<n}(x_{j_1}+\cdots+x_{j_r})^k,$$

i.e.

$$\sum_{\substack{r=0\\ r\ even}}^{n} \sum_{0\le j_1<\cdots<j_r<n} (x_{j_1}+\cdots+x_{j_r})^k = \sum_{\substack{r=0\\ r\ odd}}^{n} \sum_{0\le j_1<\cdots<j_r<n} (x_{j_1}+\cdots+x_{j_r})^k \ .$$

It follows immediately that the sets

$$A = \{x_{j_1}+\cdots+x_{j_r} \mid 0 \le r \le n, r \in 2\mathbb{N},\ 0 \le j_1 < \cdots < j_r < n\}$$

and

$$B = \{x_{j_1}+\cdots+x_{j_r} \mid 0 < r \le n, r \in 2\mathbb{N}+1,\ 0 \le j_1 < \cdots < j_r < n\}$$

have n–property.

Example 13 *Starting with $x_1 = 1, x_2 = -2, x_3 = 3, x_4 = -4, x_5 = 5$ we arrive (after removing numbers belonging to the both sets) at the sets $A = \{-6, -1, 0, 1, 7, 8\}$ and $B = \{-5, -4, 2, 3, 4, 9\}$ that have 5–property. (Zero in set A is obtained as an empty sum.)*

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A note on Candido's identity and Heron's formula

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Abstract

The square of the sum of squares of three consecutive Fibonacci numbers is twice the sum of their fourth powers. This is Candido's identity. Abstractly, it holds for any two elements and their sum in any commutative ring. Geometrically, it reveals the degeneracy of a triangle via Heron's area formula. Higher dimensional analogues via volume formulas of tetrahedra are also discussed. The identity and its cubic variant can be applied to various combinatorial and geometric formulas to obtain corresponding symmetric identities, and an algebraic application is to the polynomial Fermat's cubic equation.

Keywords: Candido's identity; Heron's formula; Fibonacci numbers

MSC: 11B39

1.1 Candido's identity and some applications

The Candido identity (named after Giacomo Candido, 1871-1941) was published in 1951, and says that the square of the sum of squares of three consecutive Fibonacci numbers is equal twice the sum of their fourth powers. Thus,

$$(F_{n-1}^2 + F_n^2 + F_{n+1}^2)^2 = 2(F_{n-1}^4 + F_n^4 + F_{n+1}^4).$$

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To prove it geometrically, recall first that the area S of a triangle ΔABC with side lengths a, b and c is given by Heron's formula from about 60 AD, but apparently Archimedes knew it some 300 years earlier. It reads as follows.

$$\begin{aligned}(4S)^2 &= (a^2+b^2+c^2)^2-2(a^4+b^4+c^4)=(2ab)^2-(a^2+b2-c^2)^2\\ &= (a+b+c)(-a+b+c)(a-b+c)(a+b-c).\end{aligned}$$

(A quick proof of Heron's formula is by using Pythagoras' theorem $\cos^2 C+\sin^2 C=1$, and cosine and sine rules: $\cos C=(a^2+b^2-c^2)/(2ab)$ and $\sin C=2S/(ab)$.) Now, from the basic Fibonacci recurrence $F_{n+1}=F_n+F_{n-1}$, it follows that the triangle whose side lengths are these numbers is degenerated. Hence, its area S is zero. By Heron's formula, the difference between the left and right side of Candido's identity is zero. This proves the identity. ■

By the same geometric argument, Candido's identity holds for any two positive numbers and their sum. For a genuine triangle, of course, we have the corresponding Candido's inequality.

In a pure algebraic setting, for every two elements x, y of any commutative ring, the Candido identity is a curious equality (and can simply be checked by expanding both sides):

$$(x^2+y^2+(x+y)^2)^2=2(x^4+y^4+(x+y)^4).$$

For three summands, $x+(y+z)=(x+y)+z$, we obtain two corresponding Candido identities etc.

Interpretations and visual proofs of the identity for real positive numbers are given in [1] and [2]. We remark that Candido's identity and the basic Fibonacci recurrence are equivalent, again by Heron's formula. Note that this identity also holds for Lucas numbers, Pell numbers, hyper-Fibonacci numbers (defined for $n, r \geq 1$ by $F_n^{(r)}=F_{n-1}^{(r)}+F_n^{(r-1)}$, and $F_n^{(0)}=F_n, F_0^{(r)}=0, F_1^{(r)}=1$, for $n, r \geq 0$), Horadam polynomial second order recurrences, and many other sequences of that type. In fact, it holds for every sequence defined by recurrence or formula of the form $x+y=z$.

A generalization of Candido's identity is the following functional equation for an unknown function f defined on positive real numbers with values also in positive reals:

$$f[f(x)+f(y)+f(x+y)]=2[f(f(x))+f(f(y))+f(f(x+y))].$$

The only solution when f is a continuous surjection with $f(0)=0$ is the squaring function (times a constant), i.e., $f(x)=Cx^2$, see [1]. Proof boils down to prove that the set $\{2^m 3^n : m, n \text{ integers}\}$ is dense on positive reals, and this follows from the fact that the sequence $\log_2 3, 2\log_2 3, 3\log_2 3, ...$ of multiples of the transcendental number $\log_2 3$ is uniformly distributed modulo 1.

Candido's identity simply transforms a recurrence or formula (automatically) in terms of sums of squares and fourth powers or in terms of other symmetric functions. For example, consider combinatorially interesting Padovan's sequence $1, 1, 1, 2, 2, 3, 4, 5, 7, 9, 12, 16, 21, \ldots$ where each member (except first three) is the sum of the second and third preceding it; $P_{n+2} = P_n + P_{n-1}$, $P_0 = P_1 = P_2 = 1$. The n-th Padovan number P_n, $n \geq 2$, is the number of ways of writing $n+2$ as an ordered sum (composition) of 2's and 3's. (Recall, F_{n+1}, $n \geq 1$, is the number of compositions of 1's and 2's whose sum is n.) In the same manner as before, we have

$$(P_{n-1}^2 + P_n^2 + P_{n+2}^2)^2 = 2(P_{n-1}^4 + P_n^4 + P_{n+2}^4).$$

As the golden ratio is attached to Fibonacci numbers, consecutive Padovan numbers ratios tend to the plastic number p (approximately 1,3247...), satisfying the cubic equation $p^3 = p+1$. Yet another combinatorial example is to apply Candido' s identity to Pascal's formula for binomial coefficients $\binom{n+1}{k} = \binom{n}{k-1} + \binom{n}{k}$ to get a symmetric expression in all three of them. So, we get "for free" the following identity:

$$\left[\binom{n}{k-1}^2 + \binom{n}{k}^2 + \binom{n+1}{k}^2\right]^2 = 2\left[\binom{n}{k-1}^4 + \binom{n}{k}^4 + \binom{n+1}{k}^4\right].$$

A geometric example is to apply Candido's identity to the Pythagorean theorem ($c^2 = a^2 + b^2$). The result is totally symmetric. So, a triangle is right if and only if the square of the sum of fourth powers of its side lengths is twice the sum of their eight powers:

$$(a^4 + b^4 + c^4)^2 = 2(a^8 + b^8 + c^8).$$

Denoting by p_n the sum of n-th powers in variables a, b and c, the Pythagorean theorem then reads as follows:

$$p_4^2 = 2p_8.$$

The form $a^2 + b^2 = c^2$ needs 8 symbols, while the above version needs only 7 symbols (5 different). Note that degenerate Heronian triangles (integer side lengths and area zero) are not accounted by parametrizations given by Brahmagupta and later by Euler (see [3]). Of course, they are parametrized by two nonnegative integers (and their sum).

1.2 The cubic Candido's identity, Fermat's equality and other applications

Heron's formula can also be written in the following way. Let $e_1 = a + b + c = 2s$ (perimeter), $e_2 = ab + bc + ca$, $e_3 = abc$, be the elementary symmetric functions of a, b and c. Then from

$$(4S)^2 = 2s(2s - 2a)(2s - 2b)(2s - 2c) = e_1(4e_1e_2 - e_1^3 - 8e_3)$$

we get that $S = 0$ if and only if $4e_1e_2 - e_1^3 - 8e_3 = 0$ (assuming non degeneracy $e_1 \neq 0$). So, $D_3(a, b, c) := (-a + b - c)(a - b + c)(a + b - c) = 0$ implies the cubic Candido's identity

$$(a + b + c)^3 + 8abc = 4(a + b + c)(ab + bc + ca).$$

This identity also makes sense in any integral domain (commutative ring without zero divisors), for elements a, b, c whose sum is not zero, but one of them is the sum of the other two. In geometric terms of the semi-perimeter s of a triangle, it can simply be written as:

$$s^3 + e_3 = se_2.$$

Hence, we have the corresponding cubic Candido identities for Fibonacci numbers, Padovan numbers, Pascal's formula, Horadam polynomials, etc. before substitution $a + b = c$.

For any triangle (genuine or degenerate) we have the cubic Candido's triangle inequality:

$$s^3 + abc \leq s(ab + bc + ca),$$

with equality if and only if the triangle is degenerate (just multiply all three triangle inequalities). Algebraically, Candido's identity $p_2^2 = 2p_4$ is equivalent to $e_1(e_1^3 - 4e_1e_2 + 8e_3) = 0$, and this follows simply by expressing power sums p_2 and p_4 in terms of e_1, e_2 and e_3.

As a combinatorial example this time, consider the sequence 1,1,2,4,9,21,51,127,323,... of Motzkin numbers M_n given by

$$(n + 2)M_n = (2n + 1)M_{n-1} + 3(n - 1)M_{n-2},$$

and $M_0 = M_1 = 1$. The Motzkin number M_{n+1} counts n-tuples of positive integers which start and end by either 1 or 2 with differences between neighbors -1,0, or 1. The quotients $M_{n+1}/M_n \to 3$ as $n \to \infty$. By the cubic Candido's identity we have (again "for free") the corresponding identity for Motzkin numbers:

$$\begin{aligned}((n+2)M_n + (2n+1)M_{n-1} + 3(n-1)M_{n-2})^3 + 24(n+2)(2n+1)(n-1)M_nM_{n-1}M_{n-2} \\ = 4[(n+2)M_n + (2n+1)M_{n-1} + 3(n-1)M_{n-2}] \\ \times[(2n^2+5n+2)M_nM_{n-1} + 3(n^2+n-2)M_nM_{n-2} + 3(2n^2-n-1)M_{n-1}M_{n-2}].\end{aligned}$$

If we apply Candido's cubic identity to the Pythagorean theorem $a^2+b^2=c^2$, now with $e_1 = a^2+b^2+c^2$, $e_2 = a^2b^2+b^2c^2+c^2a^2$, $e_3 = a^2b^2c^2$, then $s^3+e_3 = se_2$ implies the following symmetric identity of degree 6 (before substituting $a^2+b^2=c^2$):

$$(a^2+b^2+c^2)^3 + 8(abc)^2 = 4(a^2+b^2+c^2)((ab)^2+(bc)^2+(ca)^2).$$

We can apply Candido's cubic identity to the Ptolemy theorem ($ef = ac+bd$ for a circumscribed quadrilateral with side lengths a,b,c,d and diagonals e,f), and many other basic geometric facts equivalent to the Euclidean fifth postulate, but we shall skip it here.

Consider now the cubic ("Fermat") equality $a^3+b^3=c^3$ for relatively prime polynomials $a=a(x)$ etc. over integers, and at least one of the polynomials a,b,c non constant. From cubic Candido's identity $e_1^3+8e_3 = 4e_1e_2$, we have

$$(a^3+b^3+c^3)^3 + (2abc)^3 = 4(a^3+b^3+c^3)((ab)^3+(bc)^3+(ca)^3).$$

In the ring of integer polynomials we have two relatively prime polynomial factorizations into symmetric homogeneous irreducible factors of degrees 3 and 6 in variables a,b,c (before substituting $a^3+b^3=c^3$):

$$\begin{aligned}(a^3+b^3+c^3+2abc)((a^3+b^3+c^3)^2 - 2(abc)(a^3+b^3+c^3) + 4(abc)^2) \\ = 4(a^3+b^3+c^3)((ab)^3+(bc)^3+(ca)^3).\end{aligned}$$

If we write it as $PQ = 4RS$, the only possibilities are $P = kR$, $Q = lS$, where k,l are integers with $kl = 4$. For $x=0$ denote $a_0 = a(0)$ etc. Then $a_0^3+b_0^3=c_0^3$, where we may assume that a_0,b_0,c_0 are coprime integers. So, only one of them is even. Say, a_0 is even and b_0,c_0 odd. If $k=l=2$, i.e., $P=2R$, $Q=2S$, we get $2(abc)^2 = (ab)^3 + (a_3+b_3)^2$, and for $x=0$, on the left is an even number, and on the right an odd number, a contradiction. If $k=1$ (and $l=4$), then $abc=0$, say $a=0$, and this contradicts the fact that a,b,c are coprime. If $k=4$ (and $l=1$), and $k=-1$, $k=-2$ and $k=-4$, the even-odd game brings us again to absurds. The same argument works not only for cubes but also for all multiple powers of 3.

Let us only briefly recall that in general, if f, g and h are relatively prime polynomials (over complex numbers), at least one of them non constant, and such that $f^n + g^n = h^n$, then $n \leq 2$. To prove it, recall first Mason's lemma (from 1984): if $a + b = c$, where $a = a(x)$, $b = b(x)$, $c = c(x)$ are coprime polynomials, at least one of them non constant, then $\max\{\deg a, \deg b, \deg c\} < n_0(abc)$. Here $n_0(f) := \deg(\operatorname{rad} f)$, where $\operatorname{rad} f$ is the product of all distinct prime factors of the polynomial $f = f(x)$, i.e., $n_0(f)$ is the number of all distinct roots of f, and $n_0(0) := -\infty$. The "moral" of Mason's lemma is that the number of distinct prime divisors of the product of three coprime members is not very small if one of the factors is the sum of the other two. (The corresponding "abc conjecture" in number theory seems to be much more subtle.)

A quick proof of Mason's lemma is to observe that $f/\operatorname{rad} f$ divides the derivative f' (just write f as the product of powers of prime factors). From $a + b = c$ and $a' + b' = c'$, it is easy to check that $ab' - a'b = b'c - bc'$. Next, $c/\operatorname{rad} c$ divides both c and c', hence $b'c - bc'$, and similarly $b/\operatorname{rad} b$. Also, $a/\operatorname{rad} a$ divides $ab' - a'b = b'c - bc'$. Since a, b, c are coprime, so are $a/\operatorname{rad} a$, $b/\operatorname{rad} b$, $c/\operatorname{rad} c$. Therefore, their product divides $b'c - bc'$. Assume conversely that $\deg a \geq n_0(abc)$. This implies

$$\deg(abc/\operatorname{rad}(abc)) = \deg(abc) - n_0(abc) \geq \deg(abc) - \deg a = \deg(bc) > \deg(b'c - bc').$$

But only the zero polynomial (of degree $-\infty$) can be divisible with a polynomial of higher degree. So, $b'c - bc' = ab' - a'b = 0$. Since a divides ab', it follows that a divides ba', but since $\gcd(a, b) = 1$, it follows that a divides a', and this in turn implies $a' = 0$, and similarly $b' = c' = 0$, i.e., all a, b and c are constants. This contradiction proves the lemma.

Now the polynomial "FLT" follows easily, since $f^n + g^n = h^n$ implies by Mason's lemma that the degrees of f^n, g^n, h^n are less than or equal to $\deg f + \deg g + \deg h - 1$ (by assumption this is ≥ 0). Addition of three inequalities yields

$$n(\deg f + \deg g + \deg h) \leq 3(\deg f + \deg g + \deg h) - 3,$$

implying $n \leq 2$. More generally, by using Mason's lemma, it is easy to show that the polynomial Diophantine equation $fp + gq = hr$, where $2 \leq p \leq q \leq r$, can have solutions only if $(p, q, r) = (2, 2, r), (2, 3, 3), (2, 3, 4)$ or $(2, 3, 5)$.

1.3 Higher dimensional Candido's identity and concluding remarks

Now, in 3D and higher dimensions, a similar "zero-volume" method could be applied as well. Heron's formula for the volume V of an n-simplex $A_0A_1...A_n$ in terms of its edge lengths $d_{i,j} = d(A_i, A_j)$ is also known as the Cayley-Menger formula from 1928:

$$(-1)^{n+1}2^n(n!V)^2 = \det(CM_n),$$

where CM_n is the $(n+2)\times(n+2)$ matrix obtained from the $(n+1)\times(n+1)$ matrix $M = (d_{i,j}^2)$ by bordering M with a top row $(0,1,...,1)$ and a left column $(0,1,...,1)^T$; references for proof are in [4], see also [5, 6].

So, the volume vol(T) of a tetrahedron T whose basis is a triangle with edge lengths U, V and W and opposite (disjoint) to them u, v and w, respectively, is given by (Piero della Francesca, 15th century):

$$\begin{aligned}(12\mathrm{vol}(T))^2 &= (U^2+u^2)(-U^2u^2+V^2v^2+W^2w^2)+(V^2+v^2)(U^2u^2-V^2v^2+W^2w^2)\\ &\quad +(W^2+w^2)(U^2u^2+V^2v^2-W^2w^2)-(Uvw)^2-(uVw)^2-(uvW)^2\\ &\quad -(UVW)^2,\end{aligned}$$

or as Euler presented it in 1752:

$$\begin{aligned}(12\mathrm{vol}(T))^2 &= (2uvw)^2-u^2(v^2+w^2-U^2)^2-v^2(w^2+u^2-V^2)^2-w^2(u^2+v^2-W^2)^2\\ &\quad +(v^2+w^2-U^2)(w^2+u^2-V^2)(u^2+v^2-W^2).\end{aligned}$$

The polynomials on the right hand sides do not factorize (see [4]), but the $(1,1)$-minor of $\det(CM3)$, which is the squared area of the triangle with side lengths Uu, Vv and Ww factorizes. In fact, we have the following product formula for volume (see, e.g., [5] or [6]):

$$(24R\mathrm{vol}(T))^2 = (Uu+Vv+Ww)(-Uu+Vv+Ww)(Uu-Vv+Ww)(Uu+Vv-Ww),$$

where R is the circumradius of the tetrahedron T.

If one of the last three factors in the above formula is zero, then T is a circumscribed quadrilateral by Ptolemy's theorem.

There are many interesting consequences of the fact that vol$(T) = 0$. For example, if we take any point in the plane of an equilateral triangle with side length a and distances d_0, d_1 and d_2 to the vertices of the triangle, then the volume of this planar four-point configuration is zero, and the following quartic Candido type identity holds (e.g., from Euler's volume formula):

$$(a^2+d_0^2+d_1^2+d_2^2)^2 = 3(a^4+d_0^4+d_1^4+d_2^4).$$

A simple (integer) example (a, d_0, d_1, d_2) is $(8, 3, 5, 7)$, and another one is $(112, 57, 65, 73)$. If a point is taken in space, but out of the plane of the triangle, then the inequality $>$ occurs instead of equality $=$.

Similarly, if we take a point in a regular tetrahedron of edge length a, with distances d_0, d_1, d_2 and d_3 to the vertices of the tetrahedron, then we have the following Candido type identity (think of the methane molecule CH_4, where the atom C is in the center or perhaps displaced a bit from the center of the H-tetrahedron):

$$(a^2 + d_0^2 + d_1^2 + d_2^2 + d_3^2)^2 = 4(a^4 + d_0^4 + d_1^4 + d_2^4 + d_3^4).$$

This is useful in chemistry, and can serve as an equation for unknown a or one of d_i's.

In general, for a regular n-simplex with edge length a and a point in the hyperplane spanned by it, with distances to the vertices d_i for $i = 0, 1, \ldots, n$, we have (from the Cayley-Menger formula):

$$(a^2 + \sum d_i^2)^2 = (n+1)(a^4 + \sum d_i^4).$$

Note that the ordinary Candido identity is the 1-dimensional case of the this formula.

The above identity is reminiscent of Soddy's mutually kissing (tangent) spheres formula: if $n+2$ spheres of dimension $n-1$ in the Euclidean n-space kiss each other, then $(\sum c_i)^2 = n \sum c_i^2$, where $c_i = 1/r_i$ is the curvature of the i-th sphere, $i = 1, 2, ..., n+2$. In particular, for $n = 2$, this is the famous Descartes' four circle theorem from 1643. No wonder, it is also a consequence of Heron's formula.

The "zero-volume" geometric procedure can, in principle, be applied to any n-simplex. However, the Cayley-Menger polynomial is irreducible in dimension $n \geq 3$ (see [4]); in other words, there is no Heron's type product formula for volume of a simplex in terms of edges in higher dimensions, and hence no general symmetric identities of Candido's type, except in special cases as above. For a general n-simplex there are some sharp symmetric inequalities for volume V in terms of edges $d_{i,j}$. For example (see [7]),

$$2^n (n!V)^2 \leq (n+1) \left(\prod d_{i,j} \right)^{4/(n+1)},$$

with equality if and only if the simplex is regular.

In dimension 3 for a tetrahedron T there is also Kahan's product formula for volume from 1985 (available online). As before, let u, U; v, V and w, W, respectively, be pairs of opposite side lengths of T, where u, v and w have a common vertex. Then the volume $\mathrm{vol}(T)$ of T is given by:

$$(3 \cdot 2^6 \cdot uvw \cdot \mathrm{vol}(T))^2 = (-a+b+c+d)(a-b+c+d)(a+b-c+d)(a+b+c-d),$$

where $a = \sqrt{xYZ}$, $b = \sqrt{XyZ}$, $c = \sqrt{XYz}$, $d = \sqrt{xyz}$, and $X = (-U+v+w)(U+v+w)$, $x = (U-v+w)(U+v-w)$ and similarly $Y = (u-V+w)(u+V+w)$, $y = (-u+V+w)(u+V-w)$, $Z = (u+v-W)(u+v+W)$, $z = (-u+v+W)(u-v+W)$.

For instance, if T is a regular tetrahedron with side length t, then $a = b = c = 3t^3$, and $d = t^3$; next if T is a corner of a brick with edges u, v, w, then $X = x = 2vw$, $Y = y = 2uw$, $Z = z = 2uv$, and $a = b = c = d = 2uvw\sqrt{2}$, while if $u = v = w = t\sqrt{3}$, and $U = V = W = 3t$, then $a = b = c = 9t^3$ and $d = 27t^3$, and T is an equilateral triangle and its center (so, $\mathrm{vol}(T) = 0$). Let us mention here that it is an open problem ("perfect Euler's brick problem") whether there exist integers u, v, w as brick edge lengths such that plane diagonals U, V, W and space diagonal $\sqrt{u^2+v^2+w^2}$ all have integer lengths.

A Heronian tetrahedron example is $U, V, W = 25, 39, 56$ and $u, v, w = 120, 160, 153$, having face areas $area(25, 39, 56) = 420$, $area(25, 153, 160) = 1404$, $area(39, 120, 153) = 1872$, $area(56, 120, 160) = 2688$, and volume 8064. $X = 2^6 3^4 13^2$, $x = 2^6 3^2$, $Y = 2^3 3^3 13^2$, $y = 2^4 3^3$, $Z = 2^8 3 \cdot 7^2$, $z = 2^9 \cdot 3$, then $a = 2^8 3^3 7 \cdot 13\sqrt{2}$, $b = 2^9 3^4 7 \cdot 13^2$, $c = 2^9 3^4 13^2$, d= $2^9 3^3\sqrt{2}$. (U, V, W and u, v, w are length edges of a tetrahedron iff they obey all triangle inequalities and the (1,1)-minor of CM_3 has positive determinant, for a nice proof see [8].)

From six facial difference products (of three faces, not of the base UVW-triangle), as positive independent variables, we can reconstruct all six edge lengths, e.g.,

$$(2u)^2 = (Y+y)(Z+z)/(X+x),$$
$$(2U)^2 = (X(Y+y-Z-z)^2 + x(Y+y+Z+z)^2)/(Y+y)(Z+z),$$

etc.

Suppose, for instance, that in Kahan's formula $b+c+d = a$, i.e. $\sqrt{XyZ} + \sqrt{XYz} + \sqrt{xyz} = \sqrt{xYZ}$. By substituting u, v, w, U, V, W we obtain the sum of three square roots, equals also to a square root and each square root has 6 factors. The volume of T is then zero, and we have as a result of "freeing the square roots" the following polynomial identity of degree 6 (from Euler's volume expression):

$$\begin{aligned}(2uvw)^2 \quad + \quad & (v^2+w^2-U^2)(w^2+u^2-V^2)(u^2+v^2-W^2) \\ = \quad & u^2(v^2+w^2-U^2)^2 + v^2(w^2+u^2-V^2)^2 + w^2(u^2+v^2-W^2)^2.\end{aligned}$$

From the product formula it is also equivalent to

$$(-uU + vV + wW)(uU - vV + wW)(uU + vV - wW) = 0,$$

and this is again cubic Candido's identity for quantities uU, vV and wW.

An interesting special case is when opposite edges are equal. Then T is called equifacetal (or disphenoid). In this case we get the same identity as for the Pythagorean theorem, $e_1^3 + 8e_3 = 4e_1e_2$ in variables $A2$, $B2$, $C2$, where $A = u = U$ etc.

Back to Kahan's formula, $\mathrm{vol}(T) = 0$ (assuming $uvw \neq 0$) if and only if

$$D4(a, b, c, d) := (-a + b + c + d)(a - b + c + d)(a + b - c + d)(a + b + c - d) = 0.$$

In terms of elementary symmetric functions $e_1 = e_1(a, b, c, d)$, and similarly e_2, e_3, e_4, we have that $\mathrm{vol}(T) = 0$, if and only if $e_1(e_1^3 + 8e_3 - 4e_1e_2) = 16e_4$.

As a combinatorial example, consider Tribonacci numbers T_n, i.e. $0, 0, 1, 1, 2, 4, 7, 13, 24, 44, ...$ given by $T_0 = T_1 = 0$, $T_2 = 1$, $T_n + 2 = T_n{+}1 + T_n + T_{n-1}$. T_{n+2} is the number of compositions of n as sums of 1's, 2's and 3's. Note that T_{n+1}/T_n ,as $n \to \infty$, tends to the "metallic" number $t \approx 1.83929...$ which satisfies $t^3 = t^2 + t + 1$. If e_i are symmetric functions of T_j's then we get again "for free" the identity for Tribonacci numbers of Candido's type in the above form.

Finally, we describe one more volume formula where the ordinary Candido form occurs. Let $T = A_0A_1A_2A_3$ be a tetrahedron, let F_i be the face against A_i, $i = 0, 1, 2, 3$, and let (ik) be the face angle of T at the vertex A_k in F_i, $(i \neq k)$. Let R_i be the circumradius of F_i and R the circumradius of T. Then (see [9]) the volume of T is given by $3R \cdot \mathrm{vol}(T) = R_1^2R_3^2\sqrt{N}$, where $N = 2[(AB)^2 + (BC)^2 + (CA)^2] - (A^4 + B^4 + C^4)$, and $A = \sin(32)\sin(10)$, $B = \sin(31)\sin(20)\sin(12)/\sin(21)$, $C = \sin(30)\sin(12)$. Recall that the ordinary Candido identity is equivalent to $N := 2[(AB)^2 + (BC)^2 + (CA)^2] - (A^4 + B^4 + C^4) = 0$. We see that the Candido's form on the right hand side occurs in this volume formula. Clearly, $R \cdot \mathrm{vol}(T) = 0$ if and only if N is 0, because in this case R becomes infinite (and R_1 and R_3 can be considered constant).The vanishing of Candido' s form N (this time in trigonometric terms of face angles) shows that T is degenerate. A similar formula ([9]), but a bit more involved, can also be given in terms of inradii of faces, circumradius R and face angles, again in a Candido-type form.

To conclude, we see that a simple addition of two elements is via Candido's identity transformed into a symmetric equation involving sums of squares, cubes, fourth powers or other symmetric functions of summands and the sum. It is amazing that a purely algebraic formula has a simple geometric proof, and how it applies to various situations in combinatorics, algebra, geometry and analysis.

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