

SAMPLING PLANAR TANGLEGRAMS AND PAIRS OF DISJOINT TRIANGULATIONS

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ABSTRACT. A tanglegram consists of two rooted binary trees and a perfect matching between their leaves, and a planar tanglegram is one that admits a layout with no crossings. We show that the problem of generating planar tanglegrams uniformly at random reduces to the corresponding problem for irreducible planar tanglegram layouts, which are known to be in bijection with pairs of disjoint triangulations of a convex polygon. We extend the flip operation on a single triangulation to a flip operation on pairs of disjoint triangulations. Interestingly, the resulting flip graph is both connected and regular, and hence a random walk on this graph converges to the uniform distribution. We also show that the restriction of the flip graph to the pairs with a fixed triangulation in either coordinate is connected, and give diameter bounds that are near optimal. Our results furthermore yield new insight into the flip graph of triangulations of a convex n -gon with a geometric interpretation on the associahedron.

1. INTRODUCTION

A *tanglegram* consists of two rooted binary trees and a perfect matching between their leaves. They initially arose in computer science and biology [5, 7, 19]. Tanglegrams are drawn in the plane using *layouts* such as the ones shown in Figure 1. Layouts with the fewest number of crossings possible are of interest in applications such as estimating the number of horizontal gene transfers between species [27].

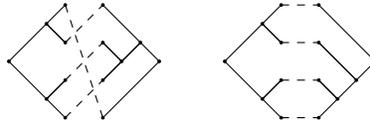


FIGURE 1. Two layouts for the same tanglegram.

Combinatorial interest has grown recently, and enumerating several variations of tanglegrams has been studied [4, 13, 24]. Algorithms for uniform sampling of tanglegrams were established in [4] and [12], and properties of random tanglegrams were studied in [15].

A tanglegram is *planar* if it has a layout with no crossings, and we refer the reader to [8, 17, 18, 24] for many interesting results about them. The second author established a characterization of all planar layouts of a planar tanglegram in [17] and then proposed the problem of efficiently sampling planar tanglegrams uniformly at random. In this paper, we consider this problem. Note that one can use the algorithms in [4] and [12] to sample tanglegrams uniformly at random

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until a planar tanglegram is generated, but results in [4] and [24] imply that planar tanglegrams are rare.

In their work enumerating planar tanglegrams, Ralaivaosaona, Ravelomanana, and Wagner [24] introduced *irreducible* planar tanglegrams, which are planar tanglegrams that cannot be constructed from smaller tanglegrams. We make this definition precise in Section 2. Let \mathcal{P} and \mathcal{I} respectively denote the set of planar and irreducible planar tanglegrams. [24, Theorem 1] gives a relation between the generating functions

$$(1.1) \quad \begin{aligned} T(x) &= \sum_{\mathcal{T} \in \mathcal{P}} x^{|\mathcal{T}|}, \\ H(x) &= \frac{1}{2}x^2 + \sum_{\mathcal{T} \in \mathcal{I}: |\mathcal{T}| > 2} x^{|\mathcal{T}|}, \end{aligned}$$

where $|\mathcal{T}|$ denotes the number of leaves in the component trees of \mathcal{T} . Their sequences of coefficients can be found at [22, A257887, A349408]. Letting $\text{Irr}(\mathcal{T})$ denote the irreducible tanglegram formed by contracting each of the smaller tanglegrams in \mathcal{T} to a pair of matched leaves, we generalize these generating functions to also account for $\text{Irr}(\mathcal{T})$ by defining

$$(1.2) \quad \begin{aligned} T(x, y) &= \sum_{\mathcal{T} \in \mathcal{P}} x^{|\mathcal{T}|} y^{|\text{Irr}(\mathcal{T})|}, \\ H(x, y) &= H(xy) = \frac{1}{2}x^2 y^2 + \sum_{\mathcal{T} \in \mathcal{I}: |\mathcal{T}| > 2} x^{|\mathcal{T}|} y^{|\mathcal{T}|}. \end{aligned}$$

We establish a generalization of the relation on $T(x)$ and $H(x)$ from [24, Theorem 1]. Note that substituting $y = 1$ recovers the original result.

Theorem 1.1. *The following holds:*

$$(1.3) \quad T(x, y) = H(T(x), y) + \frac{T(x^2)y^2}{2} + xy.$$

Using this result, we establish Theorem 3.2, which reduces the problem of generating planar tanglegrams uniformly at random to computing coefficients of $T(x, y)$ and generating irreducible planar tanglegram layouts uniformly at random. In their work enumerating planar tanglegrams, Ralaivaosaona, Ravelomanana, and Wagner [24] also established a natural bijection between irreducible planar tanglegram layouts and pairs of triangulations of a convex polygon that do not share a diagonal. We call these *pairs of disjoint triangulations*. Hence, one can instead consider the problem of generating pairs of disjoint triangulations uniformly at random.

Triangulations of a convex n -gon are one of many objects enumerated by the Catalan numbers. Sampling Catalan objects uniformly or approximately uniformly at random has been an active area of research over the last several decades. Approaches include direct methods using properties of Catalan numbers [2, 3, 25], Boltzmann sampling with the generating function relation [10], and Markov chains on flip graphs of Catalan objects [11, 20, 21]. Enumerative results suggest that pairs of disjoint triangulations are significantly more complicated than individual triangulations. In particular, there is no known simple formula in n for the number of pairs of disjoint triangulations of an n -gon, even after fixing one of the triangulations [1, 24].

We extend the flip operation on single triangulations to a new flip operation on the pairs of disjoint triangulations of an n -gon. We write \mathcal{D}_n for the graph whose vertices are pairs of disjoint triangulations and whose edges are given by flips, and we call this the *flip graph* on pairs of disjoint triangulations. The flip graph \mathcal{D}_5 is shown in Figure 2. Our flip operation implies many surprising properties for \mathcal{D}_n . In particular, we can define a *Markov chain* (X_t) from a random walk on \mathcal{D}_n . We set X_0 to be an arbitrary vertex and, for $t > 0$, choose X_t uniformly at random among the vertices adjacent to X_{t-1} .

Theorem 1.2. *For a fixed $n \geq 5$, let (X_t) be the Markov chain defined above. Then as $t \rightarrow \infty$, (X_t) converges to the uniform distribution on the vertices of \mathcal{D}_n in total variance distance.*

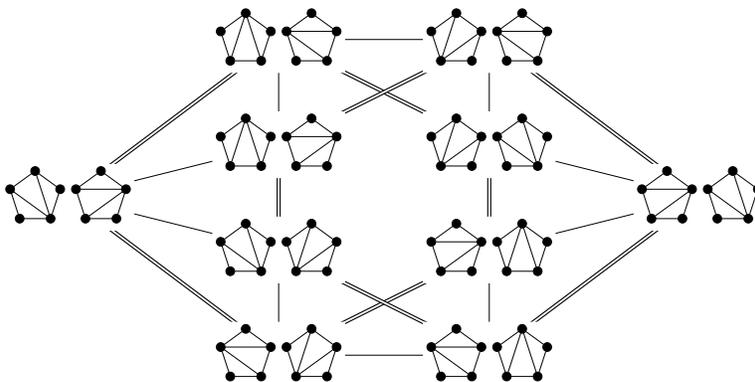


FIGURE 2. The flip graph \mathcal{D}_5 . Single lines indicate when only one triangulation is changed, and double lines indicate when both are changed.

Theorem 1.2 gives a method for near uniform sampling of pairs of disjoint triangulations. The mixing time of X_t is a topic of continued study. Our general method is similar to one used by Heitsch and Tetali to study *meanders*, which are also pairs of Catalan objects subject to some property [14]. More specifically, a meander is a pair of noncrossing matchings of $2n$ points that form a cycle, such as the one shown in Figure 3. Heitsch and Tetali also constructed a Markov chain that converges to the uniform distribution, and the mixing time of their Markov chain also remains open.

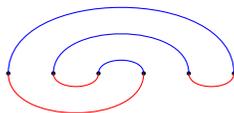


FIGURE 3. An example of a meander, with each noncrossing matching color-coded.

In order to prove Theorem 1.2, we show that \mathcal{D}_n is regular and connected. In the process, we bound the diameter of \mathcal{D}_n . In particular, we prove the following.

Theorem 1.3. *For any positive integer $n \geq 5$, the graph \mathcal{D}_n is simple, connected, and $2(n-3)$ -regular, with diameter at most $4n-16$.*

The proof of Theorem 1.3 provides novel insight into the classical flip graph of triangulations of an n -gon. Namely, we show in Theorem 4.5 that the induced subgraph of triangulations of an n -gon disjoint from some fixed triangulation is always connected. The flip graph in this case is the set of vertices and edges of the associahedron, a polytope that plays a fundamental role in algebraic and geometric combinatorics, see [6] and references therein. Our results may be rephrased within that context. The facets of the associahedron are in natural bijection with the set of diagonals of the polygon. A triangulation corresponds to a vertex of a given facet if and only if that triangulation contains the diagonal corresponding to that facet. Therefore, we have shown that for any fixed vertex v of the associahedron, the induced subgraph consisting of all vertices that do not share a facet with v is still connected with small diameter, a property that one can study for any polytope as discussed in Problem 4.

This paper is organized as follows. In Section 2, we outline background on tanglegrams and summarize relevant results in [24] on planar tanglegrams, including their connection with pairs of disjoint triangulations. In Section 3, we prove Theorem 1.1 and apply it to construct our algorithm for sampling planar tanglegrams. In Section 4, we define our flip graphs on pairs of disjoint triangulations and establish Theorems 1.2 and 1.3. We conclude in Section 5 with open problems.

2. PRELIMINARIES

A *rooted binary tree* is a tree with a distinguished vertex called the *root* where each vertex has zero or two children. We consider children to be unordered, so these are different from the plane binary trees enumerated by the Catalan numbers.

A *tanglegram* $\mathcal{T} = (L, R, \sigma)$ is formed from an ordered pair of rooted binary trees (L, R) with the same number of leaves and a perfect matching σ between the leaves of L and R . The *size* of a tanglegram, denoted $|\mathcal{T}|$, is the common number of leaves in the two trees forming the tanglegram. An isomorphism between two tanglegrams $\mathcal{T} = (L, R, \sigma)$ and $\mathcal{T}' = (L', R', \sigma')$ is an isomorphism of the underlying graphs that maps L to L' and R to R' . See [4, 19] for more details. All tanglegrams in this paper are considered up to isomorphism.

Tanglegrams are drawn in the plane using *layouts*, where L is embedded in the plane left of the line $x = 0$ with leaves on $x = 0$, R is embedded in the plane right of $x = 1$ with leaves on $x = 1$, and the matching σ is drawn using straight lines. A *crossing* in a layout is any intersecting pair of lines induced by σ . In general, a tanglegram has multiple layouts, and a tanglegram is *planar* if it has a layout in which none of the straight lines induced by σ cross. Examples are shown in Figure 4.

For a tanglegram $\mathcal{T} = (L, R, \sigma)$, suppose that for the internal vertices $u \in L$ and $v \in R$, the descendants of u and v are matched by σ . When u and v are not the roots of L and R , the subtrees rooted at v_1 and v_2 with the matching induced by σ is a *proper subtanglegram* of \mathcal{T} .

A tanglegram \mathcal{T} is *irreducible* if it contains no proper subtanglegrams. For any tanglegram \mathcal{T} , its irreducible component, denoted $\text{Irr}(\mathcal{T})$, is the tanglegram obtained by contracting each maximal proper subtanglegram to a pair of matched leaves. If \mathcal{T}' is an irreducible tanglegram, then \mathcal{T}' *extends to* \mathcal{T} if $\text{Irr}(\mathcal{T}) = \mathcal{T}'$.

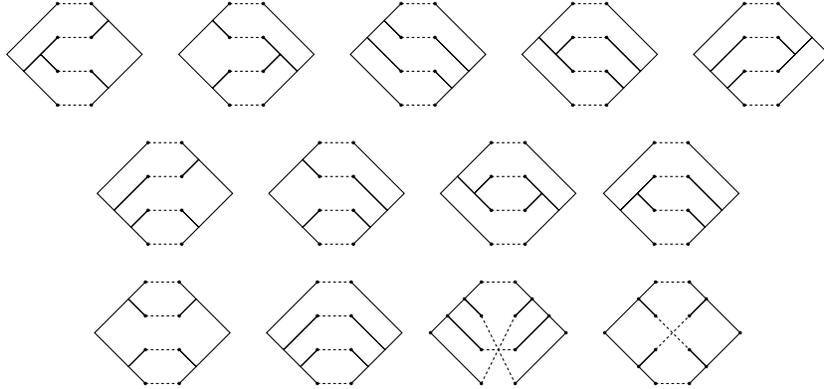


FIGURE 4. A layout for each of the 13 tanglegrams of size four.

Observe that in Figure 4, the last two tanglegrams are irreducible and not planar. Of the eleven planar tanglegrams, five are irreducible, three have an irreducible component of size two, and three have an irreducible component of size three.

We now state two results of [24]. Note that the first result can also be derived as a consequence of [17, Theorem 1.1].

Proposition 2.1. [24, Proposition 5] *Every irreducible planar tanglegram \mathcal{T} with $|\mathcal{T}| \geq 3$ has exactly two planar layouts. Moreover, the two planar layouts are mirror images of one another.*

Theorem 2.2. [24, Theorem 4] *For any $n \geq 2$, there is a bijection between the following sets:*

- the set of planar layouts of irreducible planar tanglegrams of size n , and
- the set of ordered pairs of disjoint triangulations of an $(n + 1)$ -gon.

We describe this bijection. Starting with the two plane binary trees in a planar layout of $\mathcal{T} = (L, R, \sigma)$, draw lines from the root and all leaves to infinity. Then take the plane dual. Label the region above the root in each tree as 1. In L , proceed clockwise, and in R , proceed counterclockwise. An example is shown in Figure 5.

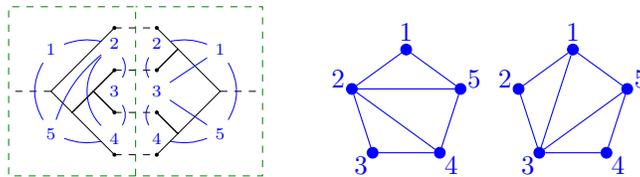


FIGURE 5. The plane dual bijection from Theorem 2.2.

3. PLANAR TANGLEGRAMS

In this section, we consider the problem of uniformly sampling planar tanglegrams. We first establish Theorem 1.1 and its consequences. We then apply these results to reduce the problem of uniformly sampling planar tanglegrams to the

corresponding problem for irreducible planar tanglegrams or their layouts in Theorem 3.2.

Recall the generating functions defined in Equations (1.1) and (1.2). We now prove Theorem 1.1, which generalizes part of [24, Theorem 1].

Proof of Theorem 1.1. We rewrite the right hand side of Equation (1.3) as

$$(3.1) \quad \left(H(T(x), y) - \frac{T(x)^2 y^2}{2} \right) + \left(\frac{T(x)^2 y^2 + T(x^2) y^2}{2} \right) + xy$$

The third summand xy accounts for the unique tanglegram where both trees consist of a single vertex. For the remaining summands, we consider those with irreducible component size two and greater than two separately.

To interpret the first summand, observe that $H(x, y) - \frac{x^2 y^2}{2}$ counts irreducible tanglegrams of size at least 3, where each term $x^k y^k$ corresponds to an irreducible planar tanglegram of size k . Proposition 2.1 implies that irreducible tanglegrams of size at least 3 have no symmetry. Consequently, given an irreducible tanglegram \mathcal{T} of size $k > 2$, fixing a layout of \mathcal{T} and replacing matched leaves from top-to-bottom with planar tanglegrams $(\mathcal{T}_i)_{i=1}^k$ produces a distinct tanglegram for each selection of $(\mathcal{T}_i)_{i=1}^k$. The generating function $T(x)^k$ counts ordered k -tuples of planar tanglegrams, and replacing pairs of matched leaves with planar tanglegrams corresponds to replacing x with $T(x)$. Hence, $H(T(x), y) - \frac{T(x)^2 y^2}{2}$ is the generating function for planar tanglegrams with $|\text{Irr}(\mathcal{T})| \geq 3$.

To interpret the second summand, tanglegrams with $|\text{Irr}(\mathcal{T})| = 2$, we must start with the unique layout for the unique tanglegram of size two and replace matched leaves with \mathcal{T}_1 and \mathcal{T}_2 . However, interchanging the order of \mathcal{T}_1 and \mathcal{T}_2 produces an isomorphic tanglegram. Observe that $T(x)^2 y^2$ double counts the cases when $\mathcal{T}_1 \neq \mathcal{T}_2$, and $T(x^2) y^2$ counts the cases when $\mathcal{T}_1 = \mathcal{T}_2$. Hence, $\frac{T(x)^2 y^2 + T(x^2) y^2}{2}$ enumerates planar tanglegrams with $|\text{Irr}(\mathcal{T})| = 2$. \square

Note that once we can efficiently compute the coefficients of $T(x)$ and $H(x)$, we can efficiently perform the composition to generate the coefficients of $T(x, y)$. Using known values of $T(x)$ and $H(x)$ from [22, A257887, A349408], we give some coefficients of $T(x, y)$ in Table 1.

n, k	2	3	4	5	6	7	8	total
2	1							1
3	1	1						2
4	3	3	5					11
5	13	9	20	34				76
6	90	46	70	170	273			649
7	747	312	360	680	1638	2436		6173
8	7040	2580	2435	3570	7371	17052	23391	63429

TABLE 1. The number of tanglegrams of size n with irreducible component size k .

We respectively use the notation t_n and $t_{n,k}$ for the coefficient of x^n in $T(x)$ and $x^n y^k$ in $T(x, y)$. We also use the notation h_n for $t_{n,n}$, which is the number of irreducible planar tanglegrams of size n . Recall that a *composition* of n is a

decomposition of n into an ordered sum of positive integers, and we use the notation $(a_i)_{i=1}^k \models n$ to denote this. The preceding theorem and proof imply the following corollary.

Corollary 3.1. *Let $2 \leq k \leq n$. The number of ways to extend a size k irreducible planar tanglegram into a size n planar tanglegram, denoted $c_{n,k}$, is independent of the irreducible planar tanglegram. Moreover,*

- (a) if n is even, then $t_{n,2} = \frac{1}{2} \left(\sum_{i=1}^{n-1} t_i t_{n-i} + t_{n/2} \right)$,
- (b) if n is odd, then $t_{n,2} = \frac{1}{2} \sum_{i=1}^{n-1} t_i t_{n-i}$, and
- (c) if $k \neq 2$, then $t_{n,k} = h_k \cdot \sum_{(a_i)_{i=1}^k \models n} t_{a_1} t_{a_2} \cdots t_{a_k}$.

Note that $c_{n,k} = t_{n,k}/h_k$.

Using these $c_{n,k}$ constants, we define a procedure for uniformly sampling planar tanglegrams that encodes the techniques from Theorem 1.1, assuming an algorithm for uniformly sampling irreducible planar tanglegram layouts. Hence, this reduces the problem of generating planar tanglegrams to generating irreducible planar tanglegrams or their layouts.

Theorem 3.2. *The following procedure generates a planar tanglegram of size $n \geq 3$ uniformly at random.*

- (1) Choose an integer $2 \leq k \leq n$ with probability $\frac{h_k c_{n,k}}{t_n}$ and generate an irreducible planar tanglegram layout \mathcal{L} of size k uniformly at random.
- (2) (a) If $k \neq 2$, select $(a_i)_{i=1}^k \models n$ with probability $\frac{t_{a_1} t_{a_2} \cdots t_{a_k}}{c_{n,k}}$ and independently generate planar tanglegrams $(\mathcal{T}_i)_{i=1}^k$ of sizes $(a_i)_{i=1}^k$ uniformly at random.
 - (b) If n is odd and $k = 2$, select $(a_1, a_2) \models n$ with probability $\frac{t_{a_1} t_{a_2}}{2c_{n,2}}$ and independently generate planar tanglegrams $(\mathcal{T}_1, \mathcal{T}_2)$ of sizes (a_1, a_2) uniformly at random.
 - (c) If n is even and $k = 2$,
 - with probability $\frac{t_{n/2}}{2c_{n,2}}$, generate a single tanglegram $\mathcal{T}_1 = \mathcal{T}_2$ of size $n/2$ uniformly at random, and
 - otherwise, select $(a_1, a_2) \models n$ with probability $\frac{t_{a_1} t_{a_2}}{\sum_{i=1}^{n-1} t_i t_{n-i}}$ and independently generate planar tanglegrams $(\mathcal{T}_1, \mathcal{T}_2)$ of sizes (a_1, a_2) uniformly at random.
- (3) In all cases, output the tanglegram corresponding to \mathcal{L} with matched leaves replaced from top to bottom by $\{\mathcal{T}_i\}_{i=1}^k$.

Proof. The definition of $c_{n,k}$ and the results of Corollary 3.1 imply that all of the necessary quantities in steps (1) and (2) sum to 1. We show that each tanglegram of size n can be generated in two ways, and each of these possibilities has probability $\frac{1}{2t_n}$.

Consider a planar tanglegram \mathcal{T} with $|\text{Irr}(\mathcal{T})| \geq 3$. To generate \mathcal{T} in the algorithm, we must first generate one of the layouts of $\text{Irr}(\mathcal{T})$ in step (1). Proposition 2.1 implies that there are two possibilities \mathcal{L}_1 and \mathcal{L}_2 , and observe that each of them has probability $\frac{h_k c_{n,k}}{t_n} \cdot \frac{1}{2h_k} = \frac{c_{n,k}}{2t_n}$ of being generated. For each \mathcal{L}_i , a unique list of tanglegrams $(\mathcal{T}_{i,j})_{j=1}^k$ must replace the matched leaves in \mathcal{L}_i from top-to-bottom to construct \mathcal{T} . Letting $a_{i,j} = |\mathcal{T}_{i,j}|$, we see in that the probability $(\mathcal{T}_{i,j})_{j=1}^k$ is generated in step (2) is given by $\frac{t_{a_1} t_{a_2} \cdots t_{a_k}}{c_{n,k}} \cdot \frac{1}{t_{a_1} t_{a_2} \cdots t_{a_k}} = \frac{1}{c_{n,k}}$. Hence, each of the

two ways of generating \mathcal{T} has probability $\frac{c_{n,k}}{2t_n} \cdot \frac{1}{c_{n,k}} = \frac{1}{2t_n}$ of being generated, so the probability \mathcal{T} is generated is $\frac{1}{t_n}$.

Next, consider a planar tanglegram \mathcal{T} with $|\text{Irr}(\mathcal{T})| = 2$. This requires first generating the unique layout \mathcal{L} for the unique planar tanglegram of size 2. If $n = |\mathcal{T}|$ is odd, then two possibilities (T_1, T_2) and (T_2, T_1) extend \mathcal{L} to \mathcal{T} . Letting $a_1 = |\mathcal{T}_1|$ and $a_2 = |\mathcal{T}_2|$, the probability of obtaining \mathcal{T} is given by

$$\frac{h_2 c_{n,2}}{t_n} \cdot \left(\frac{t_{a_1} t_{a_2}}{2c_{n,2}} \cdot \frac{1}{t_{a_1} t_{a_2}} + \frac{t_{a_2} t_{a_1}}{2c_{n,2}} \cdot \frac{1}{t_{a_2} t_{a_1}} \right) = \frac{1}{t_n}.$$

Note that $h_2 = 1$, so this term disappears in the product above.

Now consider when $n = |\mathcal{T}|$ is even. Suppose \mathcal{T} requires replacing the matched leaves in \mathcal{L} with the same tanglegram \mathcal{T}' . With probability $\frac{t_{n/2}}{2c_{n,2}} \cdot \frac{1}{t_{n/2}}$, we generate \mathcal{T}' twice in the first case of (2c), so \mathcal{T} has a

$$\frac{h_2 c_{n,2}}{t_n} \cdot \frac{t_{n/2}}{2c_{n,2}} \cdot \frac{1}{t_{n/2}} = \frac{1}{2t_n}$$

probability of being generated this way. The probability of generating \mathcal{T} by generating \mathcal{T}' twice in the second case of (2c) is

$$\frac{h_2 c_{n,2}}{t_n} \cdot \left(1 - \frac{t_{n/2}}{2c_{n,2}} \right) \cdot \frac{t_{n/2} t_{n/2}}{\sum_{i=1}^{n-1} t_i t_{n-i}} \cdot \frac{1}{t_{n/2} t_{n/2}}.$$

Using Corollary 3.1, $h_2 = 1$, and $c_{n,2} = t_{n,2}$, this simplifies to

$$\frac{c_{n,2}}{t_n} \cdot \frac{\sum_{i=1} h_i h_{n-i}}{2c_{n,2}} \cdot \frac{1}{\sum_{i=1}^{n-1} t_i t_{n-i}} = \frac{1}{2t_n}.$$

The case when \mathcal{T} requires replacing matched leaves in \mathcal{L} with two distinct tanglegrams is done using the same properties, where we note that there is no way to generate \mathcal{T} in the first case of (2c) but two ways to generate it in the second case. \square

Note that the procedure in Theorem 3.2 can be applied recursively when generating $\{\mathcal{T}_i\}_{i=1}^k$, except that the tanglegrams of size 1 and 2 should be generated directly since they are unique. For efficiency reasons, one can also directly generate all planar tanglegrams below a certain size. From this, we see that uniform sampling of planar tanglegrams can be reduced to computation of the coefficients in $T(x, y)$ and uniform sampling of irreducible planar tanglegram layouts.

4. PAIRS OF DISJOINT TRIANGULATIONS

In this section, we consider the problem of uniformly sampling pairs of disjoint triangulations, which is equivalent to uniformly sampling irreducible planar tanglegram layouts by Theorem 2.2. In Section 4.1, we construct our flip graph \mathcal{D}_n on the pairs of disjoint triangulations of an n -gon. We then establish Theorems 1.2 and 1.3 using Lemma 4.4 and Corollary 4.6. In Section 4.2, we describe the operation on irreducible planar tanglegram layouts that corresponds to flips in \mathcal{D}_n .

4.1. A flip graph on pairs of disjoint triangulations. Throughout this subsection, we fix a labeling of the convex n -gon using $[n] = \{1, 2, \dots, n\}$, and use pairs (a, b) with $a, b \in [n]$ to denote diagonals. For a triangulation T , we use the notation $(a, b) \in T$ to denote that the diagonal (a, b) is in the triangulation T .

If (a, b) is a diagonal of a triangulation T , then deleting (a, b) creates a unique quadrilateral (a, a', b, b') for some $a', b' \in [n]$. A *flip* at $(a, b) \in T$ replaces (a, b) with (a', b') , resulting in another triangulation of the n -gon. We extend the flip operation to pairs of disjoint triangulations. An example is shown in Figure 6.

Definition 4.1. Let (T_1, T_2) be an ordered pair of disjoint triangulations of an n -gon, and suppose $(a, b) \in T_i$ for some $i \in [2]$. A *flip* at $(a, b)_i \in (T_1, T_2)$ is defined as

- (a) flip $(a, b) \in T_i$, and
- (b) if the resulting diagonal (a', b') is in T_j for $j \neq i$, then flip $(a', b') \in T_j$.

When only (a) is performed, we refer to this as a *single flip*, and when both (a) and (b) are performed, we refer to this as a *double flip*.

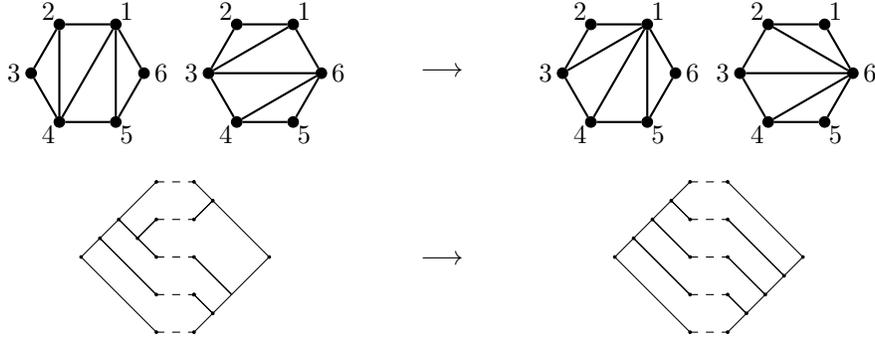


FIGURE 6. A (double) flip at $(2, 4)_1$ with the corresponding irreducible planar tanglegram layouts shown.

Lemma 4.2. Let (T_1, T_2) be an ordered pair of disjoint triangulations of an n -gon. If (T'_1, T'_2) is obtained from (T_1, T_2) by a flip at $(a, b)_i$, then (T'_1, T'_2) is also a pair of disjoint triangulations. Furthermore, (T_1, T_2) can also be obtained from (T'_1, T'_2) by some flip.

Proof. Without loss of generality, assume we flip the edge $(a, b) \in T_1$ to obtain T'_1 . If after the flip, the new diagonal (a', b') does not coincide with any diagonals of T_2 , then we are done. Note that in this case, we have that $T_2 = T'_2$, and the flip $(a', b')_2$ allows us to obtain (T_1, T_2) from (T'_1, T'_2) .

Otherwise, we flip (a', b') in the second polygon to obtain T'_2 . The resulting diagonal (a'', b'') crosses (a', b') , and hence cannot appear in T'_1 . Hence, (T'_1, T'_2) is a pair of disjoint triangulations. In this case, observe that the flip $(a'', b'')_2$ allows us to obtain (T_1, T_2) from (T'_1, T'_2) . \square

The mutual reachability between two pairs of disjoint triangulations allows us to now formally define the *flip graph on pairs of disjoint triangulations*.

Definition 4.3. Let \mathcal{D}_n denote the (undirected) graph with vertices corresponding to ordered pairs of disjoint triangulations of an n -gon and adjacency given by flips.

Observe that \mathcal{D}_3 is a single vertex graph and \mathcal{D}_4 is a path graph on two vertices. Hence, we are primarily interested in the cases $n \geq 5$.

For a given $(T_1, T_2) \in \mathcal{D}_n$, there are $2(n-3)$ diagonals on which a flip can be performed. It is not difficult to see that if $n \geq 5$, then flipping at different diagonals results in different pairs of disjoint triangulations.

Lemma 4.4. *For any integer $n \geq 5$, the flip graph \mathcal{D}_n is simple and $2(n-3)$ -regular.*

Proof. It suffices to show that for any pair (T_1, T_2) of disjoint triangulations, a flip at $(a, b) \in T_1$ and a flip at $(c, d) \in T_2$ cannot result in the same pair (T'_1, T'_2) . Let $(a', b') \in T'_1$ and $(c', d') \in T'_2$ be the diagonals obtained by flipping $(a, b) \in T_1$ and $(c, d) \in T_2$ respectively. If (T'_1, T'_2) is obtained from (T_1, T_2) by flipping $(a, b) \in T_1$, then $(a', b') = (c, d)$, and if (T'_1, T'_2) is obtained from (T_1, T_2) by flipping $(c, d) \in T_2$, then $(c', d') = (a, b)$. This implies that (a, c, b, d) is a quadrilateral in both T_1 and T_2 . Since $n \geq 5$, this implies that T_1 and T_2 share a diagonal, which is a contradiction. \square

Let \mathcal{T}_n denote the flip graph for triangulations of an n -gon. For any triangulation S of an n -gon, the subgraph of \mathcal{T}_n induced by the set of triangulations disjoint from S is denoted $\mathcal{T}_n(S)$. Pournin showed in [23] that the diameter of \mathcal{T}_n is $2n-10$ for $n > 12$. We show connectedness of \mathcal{D}_n and a linear diameter bound for \mathcal{D}_n by first showing corresponding statements for $\mathcal{T}_n(S)$.

Theorem 4.5. *Let $n \geq 5$, and let S be a triangulation of the n -gon. Then $\mathcal{T}_n(S)$ is connected, and its diameter is at most $2n-8$.*

Proof. Every triangulation contains a diagonal of the form $(i, i+2)$, so we assume without loss of generality that S contains the diagonal $(2, n)$. Let Δ denote the triangulation consisting of $\{(1, i) : 3 \leq i \leq n-1\}$, which is called a *standard triangulation* in Chapter 1 of [9]. We show that every triangulation T disjoint from S is connected to Δ by a path in $\mathcal{T}_n(S)$ of length at most $n-4$. In fact, we claim that if T contains d edges of the form $\{(1, i) : 3 \leq i \leq n-1\}$, then it is connected to Δ by a path in $\mathcal{T}_n(S)$ of length at most $n-3-d$. Note that $d \geq 1$, as $(2, n) \notin T$ implies the existence of some diagonal of the form $(1, i)$.

We prove the claim by induction on $n-3-d$. If $d = n-3$, then $T = \Delta$, and these triangulations are connected by a path of length $n-3-(n-3) = 0$ as needed. Now suppose $d < n-3$, and let $3 \leq i_1 < i_2 < \dots < i_d \leq n-1$ denote the indices such that $(1, i_j) \in T$ for all i_j . Since $d < n-3$, it must be that $i_{j+1} - i_j > 1$ for some $j \in \{1, \dots, d\}$. Consider the polygon with vertices $\{1, i_j, i_j+1, i_j+2, \dots, i_{j+1}\}$ with triangulation T_1 induced by T . Observe that T_1 cannot contain any edges of the form $(1, i)$, and since $i_j, 1, i_{j+1}$ are consecutive vertices, this can only occur if $(i_j, i_{j+1}) \in T_1$. Flipping this diagonal results in $(1, i')$ for some $i_j < i' < i_{j+1}$. Note that this diagonal $(1, i')$ cannot appear in S since S contains $(2, n)$. Hence, flipping (i_j, i_{j+1}) in T results in some triangulation T' disjoint from S that contains $d+1$ diagonals of the form $\{(1, i) : 3 \leq i \leq n-1\}$. By the inductive hypothesis, T' and Δ are connected by a path in $\mathcal{T}_n(S)$ of length at most $n-3-d-1$, and hence T is connected to Δ by a path in $\mathcal{T}_n(S)$ of length at most $n-3-d$.

Now let T_1 and T_2 be any two triangulations disjoint from S . Choosing Δ as above, we see that each T_i is connected to Δ by a path of length at most $n - 4$ in $\mathcal{T}_n(S)$, implying T_1 and T_2 are connected by a path of length at most $2n - 8$. \square

Pournin’s result for $\text{diam}(\mathcal{T}_n)$ when $n > 12$ combined with known values for $5 \leq n \leq 12$ imply that for all $n \geq 5$, we have that $\text{diam}(\mathcal{T}_n) \leq 2n - 8$. Hence, the above result implies the following statements for \mathcal{D}_n .

Corollary 4.6. *For $n \geq 5$, the flip graph \mathcal{D}_n is connected and*

$$\text{diam}(\mathcal{D}_n) \leq \text{diam}(\mathcal{T}_n) + 2n - 8 \leq 4n - 16.$$

Proof. Let $(T_1, T_2), (T_3, T_4) \in \mathcal{D}_n$. Then there is a path of length at most $\text{diam}(\mathcal{T}_n)$ in \mathcal{D}_n from (T_1, T_2) to (T_3, T) for some T disjoint from T_3 . By Theorem 4.5, there is a path from (T_3, T) to (T_3, T_4) of length at most $2n - 8$ in \mathcal{D}_n . \square

It is well known that a random walk on a regular connected graph converges to the uniform distribution in total variation distance if it is aperiodic. Aperiodicity follows from the fact that \mathcal{D}_n contains cycles of size 3 for all $n \geq 5$, which is shown using the standard triangulations in Figure 7. This implies that Theorem 1.2 follows from Theorem 1.3, which is immediate from Lemma 4.4 and Corollary 4.6.

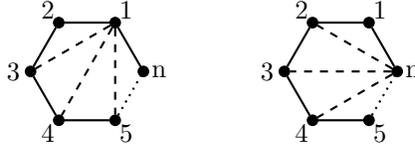


FIGURE 7. A pair of disjoint triangulations where two sequences of flips $(n, 2)_2, (2, 4)_1$ and $(n, 2)_2, (1, 3)_2, (2, 4)_1$ both result in the original pair again.

4.2. Rotations of irreducible planar tanglegram layouts. In this subsection, we establish the operation on planar layouts of irreducible planar tanglegrams that corresponds to flips in pairs of disjoint triangulations. Our operation uses the well-known rotation on plane binary trees, which is given in Figure 8. Note that our resulting correspondence is not the first of its kind, and we refer the reader to [26, Lemma 1] for one such example.

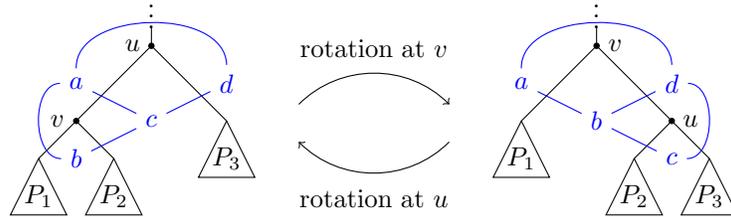


FIGURE 8. The rotation operation on rooted binary trees. A portion of the plane duals are shown in blue.

Lemma 4.7. *Let P be a rooted plane tree and T be its plane dual triangulation. The following operations correspond:*

- a rotation at vertex $v \in V(P)$, and
- a flip at the diagonal in T corresponding to the two regions separated by the edge between v and its parent.

Proof. Suppose v is the left child of its parent u . If the regions of the plane dual surrounding v and u are $\{a, b, c, d\}$ as in Figure 8, then observe that a rotation at v replaces the diagonal (a, c) in the dual with (b, d) while preserving all remaining diagonals. This is precisely a flip at the diagonal (a, c) . When v is the right child of its parent, then a similar argument applies. \square

We now generalize the rotation operation to planar layouts of irreducible planar tanglegrams. Note that any such planar layout is determined by the two component plane binary trees P_1 and P_2 , as all edges between matched leaves must be horizontal. Hence, we denote a planar layout simply as (P_1, P_2) . Furthermore, in the plane dual bijection of Theorem 2.2, if two vertices u and v form the roots of a proper subtanglegram, then the regions adjacent to their parent edges form the shared diagonal in the dual of (P_1, P_2) .

Definition 4.8. Let (P_1, P_2) be a planar layout of an irreducible planar tanglegram. A rotation at $u \in V(P_1) \cup V(P_2)$ is defined as

- (a) rotate $u \in V(P_i)$, and
- (b) if a proper subtanglegram is formed, then rotate at the vertex $v \in V(P_j)$ whose subtree forms part of a proper subtanglegram, where $j \neq i$.

Theorem 4.9. *Let \mathcal{L}_n be the graph on planar layouts of irreducible planar tanglegrams of size n with edges given by rotations. Then \mathcal{L}_n is isomorphic to \mathcal{D}_{n+1} .*

Proof. A bijection between the vertices of \mathcal{L}_n and \mathcal{D}_{n+1} is given by Theorem 2.2, so it suffices to show that the rotation and flip operations correspond appropriately. Let $(P_1, P_2), (P'_1, P'_2) \in V(\mathcal{L}_n)$ with respective plane dual pairs of triangulations $(T_1, T_2), (T'_1, T'_2) \in V(\mathcal{D}_{n+1})$. We claim that (P'_1, P'_2) can be obtained by some rotation in (P_1, P_2) if and only if (T'_1, T'_2) can be obtained by some flip in (T_1, T_2) .

Suppose (P'_1, P'_2) can be obtained from (P_1, P_2) by some rotation, which we assume without loss of generality is at some $v \in V(P_1)$. By Lemma 4.7, we have that T'_1 is obtained from T_1 by some flip. If (P'_1, P_2) does not contain any proper subtanglegrams, then the result follows. Otherwise, a proper subtanglegram in (P'_1, P_2) corresponds to a shared diagonal in (T'_1, T_2) , and we know that there is only one shared diagonal in (T'_1, T_2) . Observe that there is a unique flip in T_2 that removes the shared diagonal in (T'_1, T_2) . The rotation in P_2 described in Definition 4.8(b) removes the proper subtanglegram in (P'_1, P_2) , and hence this rotation in P_2 and the necessary flip in T'_2 must coincide. We conclude that (T'_1, T'_2) is obtained from (T_1, T_2) by some flip. A similar argument implies the converse. \square

5. OPEN PROBLEMS

Running the Markov chain on \mathcal{D}_n from Theorem 1.2 sufficiently many iterations allows for approximately uniform sampling of pairs of disjoint triangulations. Determining the number of iterations needed remains open, similar to the Markov chain in [14].

Problem 1. *Determine the mixing time of the Markov chain from Theorem 1.2 and the meanders Markov chain from [14].*

Note that a trivial upper bound for the mixing time of the Markov chain on \mathcal{D}_n is $O(|V(\mathcal{D}_n)|^2)$ [16, Proposition 10.28]. We suspect that this bound can be improved significantly because the mixing time for a random walk on \mathcal{T}_n is polynomial in n [20, 21], while $|V(\mathcal{D}_n)|$ grows rapidly with respect to n [24]. The computer data given in Table 2 supports our suspicion that $O(|V(\mathcal{D}_n)|^2)$ is not a useful upper bound for the mixing time of \mathcal{D}_n .

n	5	6	7	8	9
$ V(\mathcal{D}_n) $	10	68	546	4872	46782
iterations	3	7	14	25	39
σ_2	0.5590...	0.7287...	0.8478...	0.9512...	0.9677...

TABLE 2. For each n , the number of iterations needed for the total variation distance from the uniform distribution to be smaller than $1/4$ regardless of the initial vertex chosen, and the second largest eigenvalue of the transition matrix.

The Markov chains discussed in this paper allow for near-uniform generation of the corresponding elements. Another natural question is what properties a “typical” element has. One surprising result of [15] is that as $n \rightarrow \infty$, generating a tanglegram of size n uniformly at random becomes similar to generating two rooted plane binary trees on n leaves independently and uniformly at random. Konvalinka and Wagner used this result to establish asymptotic properties of tanglegrams.

Problem 2. *Study properties of pairs of disjoint triangulations, meanders, and planar tanglegrams generated uniformly at random. In the case of planar tanglegrams, establish analogues of results in [15].*

Known enumerative results for meanders [22, A005315] and pairs of disjoint triangulations [24] imply that these objects are not in bijection with each other. However, it is possible that other connections exist by applying certain bijections between Catalan objects.

Problem 3. *Explore connections between pairs of disjoint triangulations, meanders, and other pairs of Catalan objects satisfying some property.*

Finally, we pose a problem involving our construction of \mathcal{D}_n . Our techniques on \mathcal{D}_n can be generalized much further in the broader language of polyhedra.

Problem 4. *For a given simple polytope P , explore the graph on pairs*

$$\{(u, v) : u, v \in V(P), u \text{ and } v \text{ are not contained in the same facet}\}$$

with edges constructed in a manner similar to in \mathcal{D}_n . Determine what analogues of Theorem 1.3 hold and when this is the graph of an abstract polytope.

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