RNA SECONDARY STRUCTURES, POLYGON DISSECTIONS AND CLUSTERS

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ABSTRACT. We show that the notion of induction introduced by Cassaigne, Ferenczi and Zamboni for trees of relations arising in the context of interval exchange relations can be generalised to the case of an arbitrary number of possible edge labels. We prove that the equivalence classes of its transitive closure can still be characterised via a circular order on the trees of relations in this case. We compute the cardinalities of these equivalence classes and show that the sequence of cardinalities, for a fixed number of possible edge labels, is a convolution of a Fuss-Catalan sequence. As in the original case, the equivalence classes are in bijection with a set of pseudoknot-free secondary structures arising from the study of RNA; we show that a natural subset of this set is in bijection with a set of m-clusters (in the cluster algebra sense).

1. Introduction

In [FZ10], the authors study k-interval exchange transformations associated to the permutation $i \mapsto k+1-i$ of degree k. The behaviour of such transformations is governed by a certain class of formal languages generalising the Sturmian languages. These languages are defined using certain kinds of trees, called *trees of relations*, with edge-labels drawn from a set of three elements. The trees of relations, together with a notion of induction, are used to construct the words in the language inductively.

The combinatorics of trees of relations and the induction defined on them are studied in [CFZ10]. The transitive closure of induction on trees of relations is an equivalence relation and it is shown that the equivalence classes are characterised by a circular order on a tree of relations. It is shown in [CFZ10] that there is a bijection between an equivalence class of connected trees of relations with k vertices and maximal degree k pseudoknot-free secondary structures on 3 symbols; such structures arise in the study of RNA; see e.g. [C03]. The number of such objects is shown to be a difference of two Catalan numbers.

In this article, we show that the results of [CFZ10] can be generalised to an arbitrary number of possible edge labels on the trees of relations. In particular we generalise induction to this context and show that a suitable generalisation of the circular order is an invariant for the equivalence relation given by the transitive closure of induction. This gives a classification of the equivalence classes by k-cycles in the symmetric group of degree k.

We show further that there is a bijection between any given equivalence class and the set of maximal pseudoknot-free secondary structures with m symbols, and

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give a formula for the cardinality of these classes. This gives a formula for the total number of trees of relations with a fixed number of vertices and a fixed set of potential edge labels.

A certain nice subset of the set of maximal pseudoknot-free secondary structures on m symbols is shown to be in bijection with (m-2)-clusters in the sense of [FR05] (these generalise the clusters arising in the theory of cluster algebras [FZ02]). In fact, we give a description of our generalised induction in terms of cluster mutation.

We also give a more direct approach to computing the cardinality of the set of pseudoknot-free secondary structures, involving the direct study of the structures themselves. We further show that the sequence of cardinalities of such structures, allowing the number of vertices to vary (but fixing the number of symbols) can be regarded as an m-fold convolution of the Fuss-Catalan sequence of degree m.

We study the combinatorial situation first. In Section 2, we show that there is a bijection between the set of connected trees of relations of degree k on m symbols with a fixed circular order and the set of maximal pseudoknot-free secondary structures of degree k on m symbols, and compute the cardinality of each of these sets. In Section 3 we describe the link with (m-2)-clusters and, using this link with Fuss-Catalan combinatorics give an alternative computation of the cardinality of the set of maximal pseudoknot-free secondary structures of degree k on m symbols. In Section 4, we show the convolution result and in Section 5 we compute the total number of trees of relations of degree k on m symbols. In Section 6 we give the definition of generalised induction and show that the equivalence classes are characterised by the circular order. In Section 7 we reinterpret induction in terms of (m-2)-cluster mutation.

2. Trees of relations, secondary structures, and m-angulations

Recall that, according to [CFZ10], a shape is a tree with edges labelled by symbols +, = or -, such that no two adjacent edges have the same symbol. We define a rooted shape to be a shape together with a distinguished vertex. A tree of relations is a shape with vertices labelled $\{1, 2, ..., k\}$. Trees of relations can be rooted also. A tree of relations is also called a filling of its shape. Note that a given shape with k vertices has k! fillings.

More generally, we can consider shapes and trees of relations on m symbols of degree k in which the symbols are drawn from the set $\{S_1, \ldots, S_m\}$.

Given a shape S on m symbols, each symbol S_r determines a map (with the same name) from the set of vertices of S to itself. A vertex is fixed by S_r unless it is incident with an edge labelled S_r , in which case it is sent to the other end of the edge. Let σ_S be the composition $S_m S_{m-1} \cdots S_1$: this is a permutation of the vertices of S. We use the same definition for a tree of relations, G. We refer to σ_S (respectively, σ_G) as the *circular order* of S (respectively, G). We shall see later that in the connected case σ_G is a cycle on the vertices of a shape or tree of relations; see Lemma 5.1. For a tree of relations, G, the vertices of G are labelled with $\{1, 2, \ldots, k\}$, and in this case σ_G becomes a permutation of this set, i.e. an element of the symmetric group \mathfrak{S}_k .

We also recall from [CFZ10] the notion of a degree k pseudoknot-free secondary structure: a diagram with k vertices $1, 2, \ldots, k$, numbered clockwise in a circle. Each vertex is labelled with all of the symbols +, =, - written in order clockwise, and a collection of noncrossing links (known as links) connecting like symbols at different vertices. We again consider the natural generalisation to m symbols S_1, S_2, \ldots, S_m and call such structures degree k pseudoknot-free secondary structures on m symbols. For an example, see Figure 3(a).

Our main aim in this section is to compute the number of degree k pseudoknot-free secondary structures on m symbols. We shall also give bijective proof that this is the same as the number of connected trees of relations of degree k on m symbols with circular order $(k \ k-1 \ \cdots \ 1)$, generalising a result of [CFZ10].

The following two theorems generalise [CFZ10, 8.2,8.3,8.4].

Theorem 2.1. There is a bijection between the following sets:

- (I) The set of degree k pseudoknot-free secondary structures on m symbols.
- (II) The set of trees G of relations of degree k on m symbols such that, writing $G = \sqcup_i G_i$ as a union of connected components, we have the following:
 - (a) If $i \neq j$ and $a_1, a_2 \in G_i$, $b_1, b_2 \in G_j$, we cannot have that $a_1 > b_1 > a_2 > b_2$.
 - (b) If $a \in G_i$ for some i, then $\sigma_G(a)$ is the maximal vertex of G less than a lying in G_i (or, if no such vertex exists, it is the largest vertex of G lying in G_i).

Proof. Let Σ be a pseudoknot-free secondary structure of degree k on m symbols as in (I).

Let G be the graph with vertices $1, \ldots, k$ and edges given by the links of Σ . That is, there is an edge between vertices i and j of G labelled with symbol S_k if and only if there is a link in Σ between the instances of the symbol S_k in vertices i and j in Σ . Then G is a graph of relations with k vertices on m symbols.

Claim: G is a tree.

We prove the claim. Suppose, for a contradiction, there is a cycle

$$a_1 \xrightarrow{S_{i_1}} a_2 \xrightarrow{S_{i_2}} \dots \qquad a_{p-1} \xrightarrow{S_{i_{p-1}}} a_p \xrightarrow{S_{i_p}} a_1$$

in G, and thus a corresponding cycle in Σ . Without loss of generality, we may assume that $i_1 < i_2$. For vertices a, b, we denote by (a, b) the set of vertices c of Σ lying strictly clockwise of a and strictly anticlockwise of b.

Then $a_3 \in (a_2, a_1)$, since the link in Σ corresponding to the edge in G between a_2 and a_3 cannot cross the link in Σ corresponding to the edge in G between a_1 and a_2 .

By assumption on Σ , $i_2 \neq i_3$. If $i_2 > i_3$, there can be no path in Σ from the symbol S_{i_3} in vertex a_3 of Σ back to vertex a_1 of Σ without crossings, a contradiction, hence $i_2 < i_3$.

Repeating this argument, we see that, moving clockwise on Σ from a_1 we meet vertices a_2, a_3, \ldots, a_p in order before returning to a_1 , and that $i_1 < i_2 < \cdots < i_p$. But then the link between a_p and a_1 (on symbol S_{i_p} crosses the link between a_1 and a_2 (on symbol S_{i_1}), since $i_1 < i_p$; see Figure 1. Hence G has no cycles, and must be a tree. The claim is shown.

We next prove that (a) holds. Suppose that $i \neq j$, $a_1, a_2 \in G_i$, $b_1, b_2 \in G_j$, and $a_1 > b_1 > a_2 > b_2$. Then a_1, b_1, a_2, b_2 follow each other anticlockwise around the circle. Then, since a_1, a_2 are in the same connected component of G, there is a path in Σ from a_1 to a_2 , and similarly from b_1 to b_2 . The arrangement of a_1, a_2, b_1 and b_2 implies that these two paths cross, a contradiction. Hence no such arrangement can occur, and (a) is shown.

We next prove that (b) holds. It is enough to prove the following claim:

Claim: Let $a \in G_i$. Then $\sigma_G(a)$ is the next vertex of G_i (considered as a vertex of Σ) anticlockwise on the circle from a.

To prove the claim, we note that, by the definition of σ_G , $\sigma_G(a)$ is connected to a by a path in G:

$$a = a_1 \frac{S_{i_1}}{a_2} a_2 \frac{S_{i_2}}{a_p} \cdots \frac{S_{i_{p-1}}}{a_p} = \sigma_G(a)$$

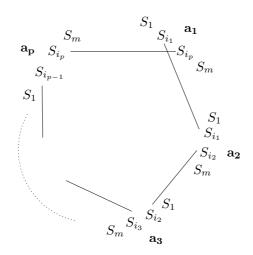


FIGURE 1. A cycle in G leads to a crossing

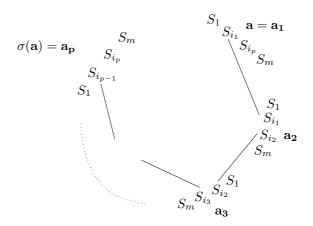


FIGURE 2. The part of Σ between a and $\sigma_G(a)$.

where $i_1 < i_2 < \cdots < i_{p-1}$. Furthermore, a_1 is not incident with any link with symbol S_r for $r < i_1$, a_p is not incident with any link with symbol S_r for $r > i_{p-1}$, and, for $2 \le j \le p-1$, a_j is not incident with any symbol S_r for $i_{j-1} < r < i_j$.

The existence of the above path implies that $\sigma_G(a)$ lies in G_i . Since $i_1 < i_2 < \cdots < i_p$ and there are no crossings, the path must go clockwise around the circle; see Figure 2. The conditions above and the fact there are no crossings imply that no vertex in $(\sigma_G(a), a)$ has a link with a vertex in $(a, \sigma_G(a))$ or with a or $\sigma_G(a)$, so these vertices are connected only amongst themselves. It follows that they do not lie in G_i and we see that (b) holds. Thus G is a tree of relations as in (II).

Conversely, suppose that we have a tree of relations G as in (II), thus satisfying (a) and (b) above. Let Σ be the secondary structure of degree k on m symbols with an link joining S_r in vertex i with S_r in vertex j if and only if there is an edge in G between vertices i and j labelled with symbol S_r . We must check that Σ can be drawn with no crossing links, i.e. that it is pseudoknot-free.

We do this by induction on the number of vertices. Suppose first that G has more than one connected component, i.e. that G is not connected. By induction,

each component G_i corresponds to a pseudoknot-free secondary structure on m symbols (on the vertices of G_i).

Suppose that we had $a_1 > a_2 \in G_i$ and $b_1 > b_2 \in G_j$ for two distinct components G_i and G_j , with links between a_1 and a_2 and b_1 and b_2 which cross in Σ . Then, going around the circle anticlockwise, starting at vertex k, we must encounter a_1, b_1, a_2, b_2 in order, or b_1, a_1, b_2, a_2 in order. Swapping G_i and G_j if necessary, we can assume we are in the first case. But then $a_1 > b_1 > a_2 > b_2$, contradicting (a). Hence Σ is pseudoknot-free.

So we are reduced to the case in which G has exactly one connected component, i.e. G is connected. Suppose that vertex k is incident with edges e_1, e_2, \ldots, e_d in G, labelled with symbols $S_{r_1}, S_{r_2}, \ldots, S_{r_d}$ where $r_1 < r_2 < \ldots < r_d$. Let the endpoints of these edges (other than k) be v_1, v_2, \ldots, v_d . Removing vertex k from G leaves precisely d trees T_1, T_2, \ldots, T_d containing vertices v_1, v_2, \ldots, v_d respectively. By (b), we know that $\sigma_G = S_m S_{m-1} \cdots S_1$ induces the permutation $(k \ k-1 \ \cdots 1)$ on the vertices of G.

We apply σ_G to vertex k, and then repeatedly apply σ_G . By its definition, each application of σ_G corresponds to following a certain path through G, i.e. passing along the edges corresponding to the symbols in the sequence S_1, S_2, \ldots, S_m in that order, when such incident edges exist. Since the edge e_1 has symbol S_{r_1} , and no edge incident with k has smaller symbol, it follows that, after the first application of σ_G , we obtain vertex $k_1 := k - 1$ in T_1 .

Since σ_G is a k-cycle, after repeated application of σ_G , we must leave T_1 . Suppose that k_2 is the number of the first vertex reached outside T_1 . Since r_2 is the minimum number of a symbol adjacent to k greater than r_1 , k_2 will lie in T_2 . Repeating this argument, we will obtain $k > k_1 > k_2 > \cdots > k_d \ge 1$ such that vertices $k_{i+1}+1,\ldots,k_i$ lie in tree T_i for $i=1,2,\ldots,d-1$. At the final step, the first vertex reached on leaving T_d must be k. Since σ_G is a k-cycle, all vertices must have been visited.

Let $k_{d+1}=0$. It follows from the above that tree T_i contains precisely vertices $k_{i+1}+1,\ldots,k_i$ for each i. Thus, the numbering of the vertices of G is first the vertices of T_d in some order, then the vertices of T_{d-1} in some order, then the vertices of T_{d-2} , and so on, ending with the vertices of T_1 and then finally k. Each T_i will correspond (by the inductive hypothesis) to a pseudoknot-free secondary structure on its vertices. Thus the vertices v_1, v_2, \ldots, v_d in G will be numbered in decreasing order. The links in Σ from K to these vertices are numbered by symbols $S_{r_1}, S_{r_2}, \ldots, S_{r_d}$, respectively, with $r_1 < r_2 < \cdots < r_d$. It follows these links do not cross each other or any of the other links in Σ . See Figure 3(a) for an example, where $v_1 = 9$, $v_1 = 1$, and $v_2 = 8$, $v_2 = 4$. Hence, Σ is pseudoknot-free and thus an object in (I) as required.

It is clear that the two maps we have constructed are inverse to each other, so the Theorem is proved. \Box

A pseudoknot-free secondary structure of degree k on m symbols is said to be maximal provided no more links can be added (i.e. any more links would have to cross the existing links in the structure).

Theorem 2.2. A pseudoknot-free secondary structure of degree k on m symbols is maximal if and only if the corresponding tree of relations is connected.

Proof. Suppose Σ is maximal, but the corresponding connected shape (which is a tree) is not connected. Then an extra edge can be added linking two components and leaving this as a tree with the same number of vertices. Applying the inverse map in the above theorem, we obtain a pseudoknot-free secondary structure with an extra link containing Σ , a contradiction. Conversely, suppose that the tree of

relations is connected but Σ is not maximal. Then an extra link can be added to Σ without introducing any crossings, since Σ is not maximal. Applying the map in the above theorem we obtain a connected shape (which is a tree) with the same number of vertices containing one more edge than the original connected tree. But it is not possible to add an edge to a connected tree and obtain a tree, so we have a contradiction. So Σ is maximal and the theorem is proved.

- **Remark 2.3.** (1) Since a connected tree on k vertices has exactly k-1 edges, a maximal pseudoknot-free secondary structure on k vertices always has k-1 links.
 - (2) In the connected case, the circular order of G is just the permutation $(k \ k 1 \ \cdots \ 1)$ and we have a bijection between the following sets:

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\{\ \textit{Maximal pseudoknot-free secondary structures of degree}\ k\ \textit{on}\ m\ \textit{symbols}\}
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{ Connected trees of relations of degree k on m symbols with circular order (k \ k-1 \ \cdots \ 1).}
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The labelling on the vertices for a tree of relations in the latter set is determined by a distinguished vertex, that labelled k, say, since σ_G then determines the labels on all the other vertices. We thus have:

Corollary 2.4. The bijection in Theorem 2.1 induces a bijection between the following sets:

- (a) Maximal pseudoknot-free secondary structures of degree k on m symbols.
- (b) Connected rooted shapes of degree k on m symbols.
- (c) Connected trees of relations G of degree k on m-symbols with circular order $(k \ k-1 \ \cdots \ 1)$.

See Figure 3(a)-(c) for an illustration of this bijection, i.e. a particular maximal pseudoknot-free secondary structure of degree 10 on 4 symbols and the corresponding objects from (b) and (c) above.

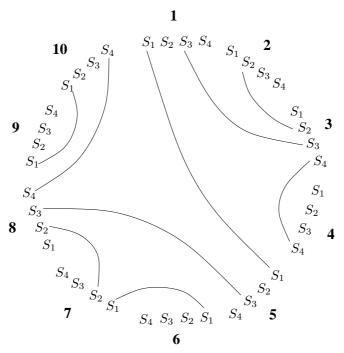
Now let P be an dk + 2-sided regular polygon. A d-diagonal in P is a diagonal joining two vertices of P which divides P into an dj + 2-sided polygon and an d(n-j) + 2-sided polygon for some j where $1 \le j \le \lceil \frac{n-1}{2} \rceil$. A maximal collection of d-diagonals of P divides P into d + 2-sided polygons. Such dissections of P are referred to as d-divisible dissections in [T06]. Taking d = m - 2, such dissections divide P into m-sided polygons, and we shall refer to them here as m-angulations of P.

We say that an m-angulation of P is diagonal-labelled if each diagonal in P is labelled with a symbol from the set $\{S_1, S_2, \ldots, S_m\}$ in such a way that the labels on the sides of each m-sided polygon in the m-angulation are S_1, S_2, \ldots, S_m in clockwise order. We say that it is rooted if there is a distinguished m-sided polygon in the m-angulation. We say that it is m-gon-labelled if the m-gons are labelled $1, 2, \ldots, k$.

In what follows, we need a bijection between diagonal-labelled m-angulations up to rotation and connected shapes of degree k on m symbols. Such a bijection in the unlabelled case (between m-angulations up to rotation and plane (m-1)-trees) is well-known; see, for example, [St99, 6.2]. Here we need a labelled version, and for convenience we give some details of how this can be done. We also note that this is a generalisation of [MSZ, 2.1] where the case m=3 is considered.

Theorem 2.5. There is a bijection between the following sets:

- (a) The set of connected shapes of degree k on m symbols.
- (b) The set of diagonal-labelled m-angulations of an (m-2)k+2-sided regular polygon up to rotation.



(a) Maximal pseudoknot-free secondary structure of degree 10 on 4 symbols.

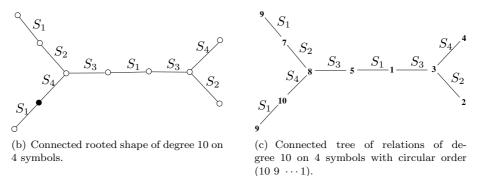


FIGURE 3. Objects corresponding to each other under the bijections in Corollary 2.4.

Proof. Given a diagonal-labelled m-angulation of an (m-2)k+2-sided polygon, take the dual graph, with a vertex in the middle of each m-sided polygon in the m-angulation and an edge between two vertices labelled S_i whenever the corresponding polygons share an edge in the dissection labelled S_i . Since the edges of a polygon in the m-angulation all have distinct labels, the same is true for the edges in the dual graph incident with a given vertex. Since there are no internal vertices in the m-angulation, there can be no cycles in the dual graph; hence it is a tree and thus a shape, clearly connected and, by construction, it is of degree k on m symbols.

Conversely, given a connected shape of degree k on m symbols, first complete it as follows. For each vertex, add extra edges with symbols not already appearing on the edges incident with the vertex. The other end of each additional edge added is a new vertex of valency 1 and is called a boundary vertex. Each original vertex has valency m in the completed shape and is referred to as an interior vertex.

Next, map the completed shape to the plane so that the edges around each vertex are labelled with the symbols S_1, S_2, \ldots, S_m in clockwise order, with all edges of unit length, and so that the edges around any given vertex are equally spaced, with an angle of $2\pi/m$ between successive edges. Note that vertices and edges may overlap. It is clear that any two such maps will be the same up to a rotation.

Next, each interior vertex determines a regular m-gon in the plane, with the midpoints of the edges in the polygon given by the mid-points of the m edges adjacent to the given vertex in the original shape. The edges in the polygon are given the same labels as the edges in the shape that they cross. The collection of regular m-gons obtained (which may also overlap) forms an m-cluster in the sense of [HPR75] (note that this is not the more modern notion of cluster introduced by Fomin-Zelevinsky [FZ02]). Then, as in [HPR75, §7] there is a homeomorphism of the plane (clearly orientation-preserving) taking the m-cluster to a (diagonal-labelled) m-angulation of P. The dissection obtained is well-defined up to a rotational symmetry of P (by the above remark concerning the map of the shape into the plane).

It is clear that this map is the inverse of the map above so the result is proved. \Box

We remark that the completion of trees considered here is quite similar to the standard completion of binary trees (i.e. a bijection from (c) to (d) in [St99, Ex 6.19]).

Corollary 2.6. There is a bijection between the following sets:

- (a) The set of connected trees of relations of degree k on m symbols with circular order $(k \ k-1 \ \cdots \ 1)$.
- (b) The set of rooted diagonal-labelled m-angulations of an (m-2)k+2-sided regular polygon up to rotation.

Proof. We use the above bijection. Given a connected tree of relations, forget the vertex labelling to obtain a connected shape, and take the corresponding diagonal-labelled m-angulation together with the distinguished m-sided polygon corresponding to the vertex in the original tree labelled k.

Conversely, given a rooted diagonal-labelled m-angulation, ignore the root and take the corresponding connected shape S. The root gives a distinguished vertex of the shape, which we label k. Then label the vertex $\sigma_S^i(k)$ by k-i for $i=1,2,\ldots,k$. It is clear that this numbering gives a tree of relations with circular order $(k \ k-1 \ \cdots 1)$.

See Figure 4 for the rooted diagonal-labelled m-angulation of an (m-2)k+2=22-sided regular polygon (up to rotation) corresponding to the connected tree of relations of degree 10 on 4 symbols with circular order (10 9 ··· 1) in Figure 3(c).

Corollary 2.7. The cardinality of each of the following sets:

- (a) The set of connected trees of relations of degree k on m symbols with circular order $(k \ k-1 \ \cdots \ 1)$;
- (b) The set of maximal pseudoknot-free secondary structures of degree k on m symbols;

is given by

$$T_{k,m} = \frac{m}{(m-2)k+2} {(m-1)k \choose k-1}.$$

Proof. Both sets have the same cardinality by Corollary 2.4 and, by Corollary 2.6, they have the same cardinality as the set of rooted diagonal-labelled m-angulations of an (m-2)k+2-sided regular polygon up to rotation. The number $S_{k,m}$ of such m-angulations without a root, with no labelling of diagonals and ignoring

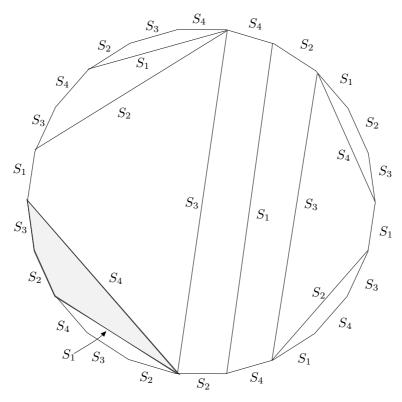


FIGURE 4. m-angulation as in Corollary 2.6(b) corresponding to the tree of relations in Figure 3(c) via the bijection in Corollary 2.6. The shaded region is the root m-gon.

rotational equivalence is well-known (see e.g. [HP91]). Let C_k^m be the kth Fuss-Catalan number of degree m:

$$C_k^m = \frac{1}{k} \binom{mk}{k-1} = \frac{1}{(m-1)k+1} \binom{mk}{k}.$$

Then

$$S_{k,m} = C_k^{m-1} = \frac{1}{(m-2)k+1} \binom{(m-1)k}{k}.$$

Since there are k m-sided polygons in an m-angulation, there are k possibilities for the root. There are m possibilities for a labelling (once one diagonal is labelled, all other diagonals in the m-angulation have determined labels using the rule that each m-gon must have its edges labelled S_1, S_2, \ldots, S_m clockwise around the boundary. Each orbit of diagonal-labelled rooted dissections under the action of the rotation group of the polygon contains (m-2)k+2 elements (the number of sides of P). Hence, we have:

$$T_{k,m} = \frac{kmS_{k,m}}{(m-2)k+2}$$

and the result follows.

Example 2.8. For m = 3, 4, 5, 6, the first few values of $T_{k,m}$ are given in the following table:

k	0	1	2	3	4	5	6
$T_{k,3}$	1	1	3	9	28	90	297
$T_{k,4}$	1	1	4	18	88	455	2448
$T_{k,5}$	1	1	5	30	200	1425	10626
$T_{k,6}$	1	1	6	45	380	3450	32886

For m = 3, we have that:

$$T_{k,3} = \frac{3}{k+2} \begin{pmatrix} 2k \\ k-1 \end{pmatrix} = C(k+1) - C(k),$$

where $C(r) = \frac{1}{r+1} \begin{pmatrix} 2r \\ r \end{pmatrix}$ is the rth Catalan number. This case is covered in [CFZ10, 7.5], and is sequence A071724 in [S110]. For m=4, we have:

$$T_{k,4} = \frac{4}{2k+2} \left(\begin{array}{c} 3k \\ k-1 \end{array} \right),$$

which is sequence A006629 in [S110]. The cases m = 5,6 do not appear in [S110].

Remark 2.9. Let $\pi \in \mathfrak{S}_k$. In 2.1-2.7, we could consider pseudoknot-free secondary structures on vertices $\pi(1), \pi(2), \ldots, \pi(k)$ (clockwise around the circle), on m symbols. Then the results 2.1-2.7 hold, with the circular order $(k \ k-1 \ \cdots \ 1)$ replaced with the circular order $\sigma = (\pi(k) \ \pi(k-1) \ \cdots \ \pi(1))$ satisfying $\sigma(\pi(i)) = \pi(i-1)$

In particular, parts (a) and (b) of Theorem 2.1 become:

- (a) If $\pi(a_1), \pi(a_2) \in G_i$ and $\pi(b_1), \pi(b_2) \in G_j$ for $i \neq j$, then we cannot have $a_1 > b_1 > a_2 > b_2$.
- (b) If $\pi(a) \in G_i$ for some i, then $\sigma_G(\pi(a))$ is the vertex $\pi(a')$ with a' less than a maximal such that $\pi(a') \in G_i$ (or, if no such vertex exists, it is $\pi(a')$ where a' is maximal such that $\pi(a')$ lies in G_i).

Furthermore, the number of trees of relations of degree k on m symbols with fixed circular order σ is given by the formula for $T_{k,m}$ in Corollary 2.7.

3. Link with Fuss-Catalan combinatorics

In this section, we show that by restricting degree k pseudoknot-free secondary structures on m symbols appropriately, we get a bijection with (m-2)-clusters of type A_{k-1} (in the sense of [FR05]). Since the number of these is well known (a Fuss-Catalan number), this, together with an appropriate bijection, gives us an alternative way of counting the total number of secondary structures, i.e. an alternative proof of Corollary 2.7.

Theorem 3.1. The following sets are all in bijection.

- (1) Degree k + 1 maximal pseudoknot-free secondary structures on m symbols with (k + 1)st vertex containing S_1 only;
- (2) Connected trees of relations G of degree k+1 on m symbols, with circular order $(k+1 \ k \cdots 1)$ and k+1 a vertex of valency 1 and edge adjacent to it labelled S_1 ;
- (3) Connected rooted shapes with k + 1 vertices on m symbols and only one edge, labelled S_1 , adjacent to the root;
- (4) m-angulations of a (m-2)k+2-sided regular polygon;
- (5) Connected rooted shapes with k vertices on m symbols and no edge labelled S₁ adjacent to the root;
- (6) rooted complete (m-1) plane trees with k internal vertices;
- (7) (m-2)-clusters (in the sense of [FR05]) of type A_{k-1} , i.e. maximal simplices of the (m-2)-cluster complex of type A_{k-1} as considered in [FR05].

Proof. (1) \leftrightarrow (2): This is a restriction of the bijection in Remark 2.3. The fact that vertex k+1 contains only the symbol S_1 corresponds to the fact that vertex k+1 in the tree has only one edge incident with it, labelled S_1 .

- $(2)\leftrightarrow(3)$: To go from an object in (2) to an object in (3), take vertex k+1 as the root and forget the labelling. For the inverse map, the condition on the circular order, σ_G , in (2) determines the labelling, starting from k+1 corresponding to the root.
- $(3) \leftrightarrow (4)$: Restricting Theorem 2.5 gives a bijection between the objects in (3) and the set of rooted diagonal-labelled m-angulations of an (m-2)(k+1)+2-sided regular polygon up to rotation such that the root polygon has only one edge incident with another polygon and that edge is labelled S_1 . Removing the root polygon gives (via an orientation-preserving homeomorphism) a rooted diagonal-labelled m-angulation of an (m-2)k+2-sided regular polygon up to rotation with a fixed boundary edge labelled S_1 . Since that edge determines the rest of the diagonal-labelling, we obtain an m-angulation of an (m-2)k+2-sided regular polygon up to rotation, with a distinguished boundary edge. The distinguished boundary edge allows us to always choose a representative in the rotation class with that boundary edge in a fixed position. So we obtain an m-angulation of an (m-2)k+2-sided regular polygon, i.e. an object as in (4).
- $(3)\leftrightarrow(5)$: Choose an object in (3), and let e be the edge labelled S_1 , incident with the root. Let the new root be the other vertex incident with e, then delete the old root and the edge e. We obtain a new rooted shape on k vertices with S_1 not labelling any edge incident with the new root. To go back, given an object in (5), add a new edge incident with the root and label it S_1 . The other end is a new vertex which becomes the new root.
- $(5)\leftrightarrow(6)$: Given an object in (5), first complete it as in the second paragraph of Theorem 2.5. Embed it in plane using the cyclical order $S_1, S_2, \ldots, S_m, S_1$ of the edges around each vertex. Using the same root, we obtain in this way a rooted completed plane m-1-tree.

To go back: given an object in (6), let the parental edge of a vertex be the edge between it and its parent. Then, given a vertex with parental edge labelled S_j , label the edges to its children clockwise from the parental edge in the order: $S_{j+1}, S_{j+2}, \ldots, S_m, S_1, \ldots, S_{j-1}$. Finally, remove any boundary vertices (except the root, which is regarded as an internal vertex).

$$(4)\leftrightarrow(7)$$
: See [FR05].

Parts (3) and (5) of Theorem 3.1 can be regarded as a generalisation of Proposition [CFZ10, 7.5] and the remark following it.

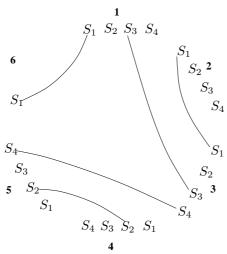
Figure 5 gives examples of objects corresponding to each other under the above bijections. For (g), we use the numbering of the vertices of the dodecagon anti-clockwise, P_1, P_2, \ldots, P_{12} , from the root edge at the bottom of the figure in (d). Following [FR05, 5.1], we see that the 2-snake consists of diagonals linking pairs of vertices (P_1, P_{10}) , (P_{10}, P_3) , (P_3, P_8) and (P_8, P_5) , corresponding to the negative simple roots $-\alpha_1^1$, $-\alpha_2^1$, $-\alpha_3^1$ and $-\alpha_4^1$, respectively. This allows the corresponding 2-cluster to be read off the 4-angulation as in [FR05, 5.1]. Here $\alpha_i + \cdots + \alpha_j$ is denoted by α_{ij} .

As previously remarked, the number of objects in (4) is known (see e.g. [HP91]) and is given by the Fuss-Catalan number C_k^{m-1} . So we have:

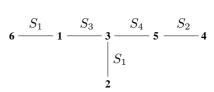
Theorem 3.2. The number of objects in each of the above is

$$S_{k,m} = C_k^{m-1} = \frac{1}{k} \begin{pmatrix} (m-1)k \\ k-1 \end{pmatrix} = \frac{1}{(m-2)k+1} \begin{pmatrix} (m-1)k \\ k \end{pmatrix}.$$

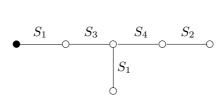
(Note that this is not new for (4), (6) and (7)).



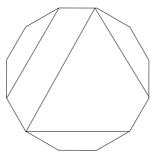
(a) Degree 6 maximal pseudoknot-free secondary structure with 6th vertex containing S_1 only



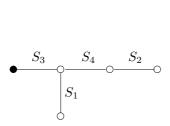
(b) Connected tree of relations of degree 6 on 4 symbols with circular order (6 5 4 3 2 1) with 6 a vertex of valency 1 connected to an edge with symbol S_1



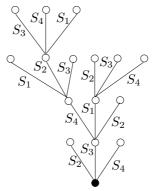
(c) Connected rooted shape of with 6 vertices on 4 symbols and only one edge, labelled S_1 , adjacent to the root.



(d) m-angulation of an (m-2)k+2=12-sided regular polygon (we take the root to correspond to the edge at the bottom of the diagram).



(e) Connected rooted shape with 5 vertices on 4 symbols with no edge labelled S_1 adjacent to the root.



(f) rooted complete ternary plane tree with 5 internal vertices.

 $\alpha_1^2, \alpha_{14}^2, \alpha_4^2, \alpha_{34}^1$ (g) 2-cluster of type A_4

FIGURE 5. Objects corresponding to each other under the bijections in Theorem 3.1.

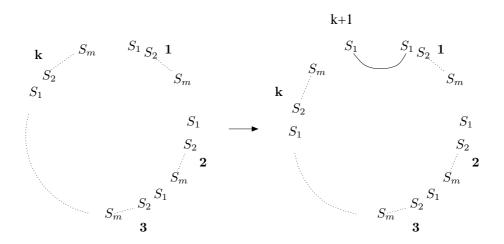


FIGURE 6. The case with no link incident with S_1 in vertex 1.

Example 3.3. For m = 3, 4, 5, 6, the values of $S_{k,m}$ for small k are given in the following table for convenience:

k	0	1	2	3	4	5	6
$S_{k,3}$	1	1	2	5	14	42	132
$S_{k,4}$	1	1	3	12	55	273	1428
$S_{k,5}$	1	1	4	22	140	969	7084
$S_{k,6}$	1	1	5	35	285	2530	23751

The case m=3, the Catalan numbers, is considered in [CFZ10, 7.5] See [Sl10], sequences A000108, A120588. The case m=4 is sequence A001764, the case m=5 is sequence A002293 and the case m=6 is A002294.

We now give a quadratic formula for $T_{k,m}$ (the number of connected trees of relations of degree k on m symbols) in terms of the $S_{l,m}$ (the number of m-angulations of an (m-2)l+2-sided regular polygon) with l varying. This allows us to give an alternative proof of the formula for $T_{k,m}$ (Corollary 2.7).

Theorem 3.4. There is a bijection between the set of maximal pseudoknot-free secondary structures of degree k on m symbols and the disjoint union of

- (a) The maximal pseudoknot-free secondary structures of degree k+1 on m symbols with vertex k+1 having symbol S_1 only and
- (b) The disjoint union for v = 2, ..., k of the set of pairs with the first consisting of a maximal pseudoknot-free secondary structure of degree v on m symbols with vertex v having symbol S_1 only and the second element consisting of a maximal pseudoknot-free secondary structure with degree k v + 2, vertex k v + 2 having symbol S_1 only.

Proof. Partition the set of maximal pseudoknot-free secondary structures Σ of degree k on m symbols by

- (a) whether there is a link in Σ incident with S_1 in vertex 1 and
- (b) if there is such a link, by the vertex $v, 2 \le v \le k$, of its other end.

The structures with no such link are in bijection with maximal pseudoknot-free secondary structures of degree k+1 on m symbols with vertex k+1 having symbol S_1 only (the bijection adds a new vertex, k+1 with symbol S_1 only and a link from S_1 in Σ , vertex 1, to vertex k+1). See Figure 6.

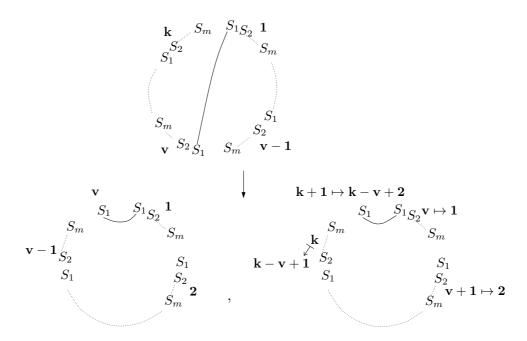


FIGURE 7. The case with an link incident with S_1 in vertex 1.

Given a structure Σ with a link incident with S_1 in vertex 1, we obtain a maximal pseudoknot-free secondary structure of degree v on m symbols with vertex v having S_1 only as a symbol, by restricting to vertices $1, \ldots, v-1$ and symbol S_1 of vertex v.

We obtain a maximal pseudoknot-free secondary structure of degree k-v+2 with only symbol S_1 in degree k-v+2 by considering the remainder of Σ not lying in the restriction above, adding the symbol S_1 to the vertex v, renumbering the vertices $1, \ldots, k+1-v$ and then following the same procedure as in the case when there is no link incident with S_1 in vertex 1. See Figure 7.

It is clear that this pair determines Σ , and the Theorem follows.

Corollary 3.5. The number of pseudoknot-free secondary structures of degree k on m symbols is given by

$$T_{k,m} = \sum_{v=1}^{k} C_{v-1}^{m-1} C_{k+1-v}^{m-1} = \sum_{v=1}^{k} S_{v-1,m} S_{k+1-v,m}.$$

Proof. This follows immediately from Theorem 3.4, with the first term (v = 1) corresponding to the case where there is no link incident with symbol S_1 in vertex 1 of the pseudoknot-free secondary structure of degree k.

Lemma 3.6. [GKP94, Eq. 5.63]

Let $n, r, s, t \in \mathbb{Z}$, with $n \geq 0$. Then we have:

$$\sum_{k=0}^{n} \frac{r}{tk+r} \cdot \frac{s}{t(n-k)+s} \begin{pmatrix} tk+r \\ k \end{pmatrix} \begin{pmatrix} t(n-k)+s \\ n-k \end{pmatrix} = \frac{r+s}{tn+r+s} \begin{pmatrix} tn+r+s \\ n \end{pmatrix}$$

(If a denominator factor vanishes, the formula still makes sense by cancelling it with an appropriate factor in the numerator of a binomial coefficient.) \Box

Note that the formula holds in greater generality but we shall not need it. We now have an alternative proof of Corollary 2.7:

Theorem 3.7. Fix integers $m \ge 1, k \ge 0$. The cardinality of the set of maximal pseudoknot-free secondary structures of degree k on m symbols is given by

$$T_{k,m} = \frac{m}{(m-2)k+2} \begin{pmatrix} (m-1)k \\ k-1 \end{pmatrix}.$$

Proof. By Corollary 3.5 we have that

$$T_{k,m} = \sum_{v=0}^{k-1} S_{v,m} S_{k-v,m} = \sum_{v=0}^{k} S_{v,m} S_{k-v,m} - S_{k,m},$$

since $S_{0,m} = 1$. Hence, using Lemma 3.6, we have:

$$\begin{split} T_{k,m} &= \sum_{v=0}^k \frac{1}{(m-1)v+1} \binom{(m-1)v+1}{v} \frac{1}{(m-1)(k-v)+1} \binom{(m-1)(k-v)+1}{k-v} \\ &- S_{k,m} \\ &= \frac{2}{(m-1)k+2} \binom{(m-1)k+2}{k} - \frac{1}{(m-1)k+1} \binom{(m-1)k+1}{k} \\ &= \frac{2}{(m-1)k+2} \cdot \frac{(m-1)k+2}{(m-2)k+2} \binom{(m-1)k+1}{k} - \frac{1}{(m-1)k+1} \binom{(m-1)k+1}{k} \\ &= \frac{2}{(m-2)k+2} \binom{(m-1)k+1}{k} - \frac{1}{(m-1)k+1} \binom{(m-1)k+1}{k} \\ &= \left(\frac{2}{(m-2)k+2} - \frac{1}{(m-1)k+1}\right) \binom{(m-1)k+1}{k} \\ &= \left(\frac{2}{(m-2)k+2} - \frac{1}{(m-1)k+1}\right) \frac{(m-1)k+1}{k} \binom{(m-1)k}{k-1} \\ &= \frac{((m-1)k+1)(2((m-1)k+1) - ((m-2)k+2))}{k((m-2)k+2)((m-1)k+1)} \binom{(m-1)k}{k-1} \\ &= \frac{m}{(m-2)k+2} \binom{(m-1)k}{k-1}, \end{split}$$

as required.

4. Convolution

In this section we show that the sequence $T_{k,m}$, $k=1,2,\ldots$ can be regarded as an m-fold convolution of the sequence $S_{k,m}$, $k=0,1,2,\ldots$

Lemma 4.1. The following sets are in bijection:

{ Maximal pseudoknot-free secondary structures of degree k+1 on m symbols in which there is a link between vertex 1 and vertex k+1 with symbol S_r }

{ Maximal pseudoknot-free secondary structures of degree k+1 on m symbols in which there is a link between vertex 1 and vertex k+1 with symbol S_1 }

Proof. Given a structure in the first set, note that there can be no links incident with vertex 1 with symbol S_t with t < r and no links with vertex k+1 with symbol S_t with t > r (since the structure is pseudoknot-free). Similarly, given a structure in the second set, there can be no links incident with vertex k+1 with symbol S_t with t > 1. It follows that moving an element Σ of the first set r-1 steps to the left, each step moving each link one symbol to the left in the diagram, gives a pseudoknot-free secondary structure Σ' of degree k+1 on m symbols in which there is a link between vertex 1 and vertex k+1 with symbol S_1 . If this structure was not maximal, an extra link could be added to it without introducing any crossings.

Shifting this extra link back r-1 steps to the right would give an extra link that could be added to Σ without introducing any crossings, a contradiction to the maximality of Σ . Hence Σ' is a structure in the second set and we get a map from the first set to the second set. It is clear that the inverse of this map is shifting r-1 steps to the right.

We note that removing symbols S_2, S_3, \ldots, S_m from vertex k+1 from an element of the second set makes no difference, since vertex k+1 can only have a link to vertex 1 with symbol S_1 by the pseudknot-free condition.

Corollary 4.2. The number of maximal pseudoknot-free secondary structures of degree k+1 on m symbols in which there is a link between vertex 1 and vertex k+1 with symbol S_r is equal to $S_{k,m}$.

Proof. Use Lemma 4.1 and Theorem 3.1.

Proposition 4.3. Let $S_{k,m}, T_{k,m}$ be as above and set $k \geq 1$. Then

$$T_{k,m} = \sum_{\substack{k_1 \ge 0, \dots, k_m \ge 0, k_1 + \dots + k_m = k - 1}} S_{k_1,m} S_{k_2,m} \cdots S_{k_m,m},$$

i.e. the sequence $T_{1,m}, T_{2,m}, \ldots$ is the m-fold convolution of the sequence $S_{0,m}, S_{1,m}, \ldots$

Proof. Let Σ be a maximal degree k pseudoknot-free secondary structure on m symbols with corresponding connected shape S (which is a tree). Recall (see Remark 2.3) that $\sigma_S(1) = k+1$, i.e. applying the symbols S_1, S_2, \ldots, S_m in order to the vertex 1 takes us from 1 to k+1. Suppose that applying symbol S_j takes us from vertex i to vertex $i+k_j$ for $j=1,2,\ldots,m$. Note that $k_j \geq 0$ for all j by the pseudoknot-free condition. We see that Σ corresponds to the joining of m maximal pseudoknot-free secondary structures on m symbols Σ_1,\ldots,Σ_m , where Σ_j has degree k_j+1 , and in which there is a link between vertex 1 and vertex k_j+1 in Σ_j with symbol S_j . Note that we must have $k_1+\cdots+k_m=k-1$. Thus we have a bijection between maximal degree k pseudoknot-free secondary structures on m symbols and such m-tuples. The formula in the proposition follows from this and Corollary 4.2.

5. The total number of trees of relations

In Section 2 we counted the number of trees of relations with a fixed circular order. We now would like to count the total number of connected trees of relations of degree k with m symbols, that is with any circular order. By Remark 2.9, the number of trees of relations with a fixed circular order σ (if σ is a k-cycle) is also given by

$$T_{k,m} = \frac{m}{(m-2)k+2} \begin{pmatrix} (m-1)k \\ k-1 \end{pmatrix}$$

We also have:

Lemma 5.1. Let G be a connected tree of relations of degree k on m symbols. Then the circular order σ_G of G is a k-cycle.

Proof. This is clearly true if k=1 or 2. Suppose it holds for smaller values of k. Let v be a vertex of G which is not a leaf. Suppose that v is incident with edges e_1, e_2, \ldots, e_d in G, labelled with symbols $S_{r_1}, S_{r_2}, \ldots, S_{r_d}$ respectively, where $r_1 < r_2 < \cdots < r_d$. Let the end-points of these edges (other than v) be v_1, v_2, \ldots, v_d . Removing v from G leaves d subtrees G'_1, G'_2, \ldots, G'_d incident with v_1, v_2, \ldots, v_d respectively. Let G_i be the subtree G'_i with v and v and v reattached to v.

By the inductive hypothesis the σ_{G_i} are all cycles. Hence, repeatedly applying σ_{G_1} to v cycles through the vertices of G_1 . Since $\sigma_G = \sigma_{G_1}$ on all vertices of G_1 except $w = \sigma_{G_1}^{-1}(v)$, repeatedly applying σ_G also cycles through all the vertices of G_1 . Since r_2 is minimal such that S_{r_2} is a symbol on an edge incident with v with $v_2 > v_1$, $v_3 = v_4$ will lie in $v_3 = v_3 = v_3$. In fact $v_3 = v_4 = v_3 = v_3$, since in $v_3 = v_4 = v_3 = v_4$ is not incident with any edge labelled with a symbol other than $v_3 = v_4 = v_4 = v_4$. Repeatedly applying $v_3 = v_4 = v_4 = v_4$. Repeating this argument, we see that repeatedly applying $v_3 = v_4 = v_4 = v_4$. Repeating this argument, we see that repeatedly applying $v_3 = v_4 = v_4 = v_4$. Then through $v_4 = v_4 = v_4$ in order before eventually returning to $v_4 = v_4 = v_4$.

(Note that it follows that the circular order on a connected shape is also a cycle.) We thus see that the number of possible circular circular orders of connected trees of relations of degree k on m symbols is the number of k-cycles in \mathfrak{S}_k , i.e. (k-1)!. It follows that:

Proposition 5.2. The total number of connected trees of relations of degree k on m symbols is

$$U_{k,m} = \frac{m((m-1)k)!}{((m-2)k+2)!}$$

Proof. By the above discussion and Lemma 5.1, we have:

$$T_{k,m}(k-1)! = \frac{m}{((m-2)k+2)} \frac{((m-1)k)!}{(k-1)!((m-2)k+1)!} (k-1)!$$
$$= \frac{m((m-1)k)!}{((m-2)k+2)!}.$$

Example 5.3. For m = 3, 4, 5, 6, we give below some values of $U_{k,m}$ for small k.

k	1	2	3	4	5	6
$U_{k,3}$	1	3	18	168	2160	35640
$U_{k,4}$	1	4	36	528	10920	293760
$U_{k,5}$	1	5	60	1200	34200	1275120
$U_{k,6}$	1	6	90	2280	82800	3946320

We note that none of these sequences appears in [Sl10].

Putting together the results of the previous sections with the above discussion, we have:

Corollary 5.4. There are bijections between the following sets:

- (1) Pairs consisting of a rooted diagonal-labelled m-angulation of degree k up to rotation and a k-cycle;
- (2) (m-gon)-labelled, diagonal-labelled m-angulations with k m-gons up to ro-tation;
- (3) Connected trees of relations of degree k with m symbols.

All the above sets have cardinality:

$$U_{k,m} = \frac{m(((m-1)k)!)}{((m-2)k+2)!}.$$

Proof. The connected trees of relations of degree k with m symbols with a fixed circular order are in bijection with rooted diagonal-labelled m-angulations of degree k up to rotation by Corollary 2.6 (see also Remark 2.9). Thus mapping a tree of relations to its corresponding m-angulation together with the circular order of the

tree gives a bijection between (3) and (1), using Lemma 5.1. To go between (2) and (3), argue as in Theorem 2.5 (the m-gon labelling of the m-angulation corresponds to the vertex-labelling of the tree of relations).

6. Generalised Induction

In this section we give the definition of our generalised induction on trees of relation with k vertices and m symbols, generalising the induction of a tree of relations with k vertices and 3 symbols defined in [CFZ10]. The induction in [CFZ10] leads in [FZ10] to the construction of new languages generalising the Sturmian languages, used to study k-interval exchange transformations. Induction generates new trees of relations starting with a given one, and the transitive closure is an equivalence relation. We show that the circular order is an invariant, giving rise to a classification of the equivalence classes by k-cycles in \mathfrak{S}_k .

Given a tree of relations G and integers $i, j \in \{1, ..., m\}$ we define a maximal $S_i - S_j$ chain B to be a (linear) subtree of G containing only symbols S_i and S_j such that no other edges incident to B are labelled by S_i or S_j .

Definition 6.1. Let G be a tree of relations with k vertices and m symbols S_1, S_2, \dots, S_m . Fix $i, j \in \{1, \dots, m\}$ with i < j. Let B be a maximal $S_i - S_j$ chain. Define $R_{i,j}^B(G)$ to be the tree of relations obtained from G by

- first removing all subtrees in the complement of the maximal chain B
- interchanging the vertices of each edge of B labelled by S_j
- interchanging the symbols S_i and S_j on the whole maximal chain B
- reattaching the previously removed subtrees to B at the vertices with the same label they were removed from.

Similarly, define $L_{i,j}^B(G)$, where in the second bullet point in the above definition we interchange the vertices of each edge labelled by S_i rather than those labelled by S_j . We also set $R_i^B := R_{i,i+1}^B$ and $L_i^B := L_{i,i+1}^B$ and we will write R_i and L_i if B is clear from the context.

Lemma 6.2. Let $i, j \in \{1, ..., m\}$ with i < j and B be a maximal $S_i - S_j$ -chain with no incident edges labelled by S_{i+1}, \ldots, S_{j-1} . Then the induction $R_{i,j}^B(G)$ is a product of inductions of the form R_l for l = i, i + 1, ..., j - 1.

Proof. Suppose first that B has the following form:

$$a_1 - \frac{S_i}{a_2} a_2 - \frac{S_j}{a_3} a_3 - \frac{S_i}{a_4} a_4 \cdots a_{r-1} - \frac{S_i}{a_r} a_r$$
. Then $R_{i,j}^B(G)$ is the chain

$$B' = a_1 \frac{S_j}{S_j} a_3 \frac{S_i}{S_j} a_2 \frac{S_j}{S_j} a_5 \frac{S_i}{S_j} a_4 \dots a_{r-2} \frac{S_j}{S_j} a_r$$
.

On the other hand, applying R_i , R_{i+1} , ..., R_{j-2} , in order (in each case to all the maximal chains of appropriate type contained in B), we obtain the maxi-

mal
$$S_{j-1} - S_j$$
-chain $a_1 \xrightarrow{S_{j-1}} a_2 \xrightarrow{S_j} a_3 \xrightarrow{S_{j-1}} a_4 \cdots a_{r-1} \xrightarrow{S_{j-1}} a_r$. Next, apply R_{j-1} to the whole chain B . Then, applying $R_{j-2}, R_{j-3}, \ldots, R_i$ in decreasing order (in each case to all the maximal chains of appropriate type contained in B) gives the chain B' .

The proof works in a similar way for the other configurations of maximal $S_i - S_j$ chains, i.e. the chains of the form

$$a_1 \xrightarrow{S_i} a_2 \xrightarrow{S_j} a_3 \xrightarrow{S_i} a_4 \qquad \cdots \qquad a_{r-1} \xrightarrow{S_j} a_r$$

and

$$a_1 \xrightarrow{S_j} a_2 \xrightarrow{S_i} a_3 \xrightarrow{S_j} a_4 \qquad \dots \qquad a_{r-1} \xrightarrow{S_j} a_r$$

Remark 6.3. (1) In the above proof, we may replace the inductions R_l with inductions L_l for l = i, i + 1, ..., j - 1.

- (2) If we replace R_{j-1} with L_{j-1} in the above proof we obtain the induction $L_{i,j}^B(G)$ instead.
- (3) Induction can also be defined on shapes: For a shape with n vertices, choose an arbitrary filling, apply induction, and then remove the filling. It is clear that this is independent of the filling chosen.
 - (4) The inductions $R_{i,j}^{B}$ and $L_{i,j}^{B}$ are mutually inverse maps.

Definition 6.4. Call two trees of relations G, G' induction equivalent if there is a sequence of inductions taking G to G', either of the form L_i , for $1 \le i \le m-1$ or of the form R_i , for $1 \le i \le m-2$. Clearly this is a reflexive relation. It is symmetric since L_i and R_i are inverse maps and it is easy to see that it is transitive. Hence it is an equivalence relation. We write $\Gamma(G)$ for the equivalence class containing G.

The inductions R_i and L_i and the above notion of induction equivalence are the ones that behave well with respect to the circular order, as we shall see below. However, we shall also denote by $\Gamma_{gen}(G)$ the equivalence class of G under the equivalence given by the more general inductions $R_{i,j}$ and $L_{i,j}$.

Proposition 6.5. Let G be a tree of relations. There exists a tree of relations G_* containing only symbols S_1 and S_m and a sequence of inductions, each of the form $R_{i,j}$ (with $j \leq m-1$) or of the form $L_{i,j}$ (with $i \geq 2$) taking G to G_* .

Proof. We first show that there exists tree of relations G_2 induction equivalent to G with no symbol S_2 in G_2 , by removing the symbols S_2 one by one. Firstly remove all edges with symbols S_4, \ldots, S_m and call the resulting tree \widetilde{G} . By [CFZ10, 5.2] there exists a sequence of inductions of the form $R_{1,2}$ and $L_{2,3}$ taking \widetilde{G} to a tree of relations \widetilde{G}_2 with no edge labelled S_2 . Let G_2 be the tree \widetilde{G}_2 with the detached edges reattached (to the vertices with the same label). Since none of the detached edges are labelled with S_1, S_2 , or S_3 this sequence of inductions also takes G to G_2 by identifying maximal chains in \widetilde{G} with corresponding maximal chains in G.

Suppose we have shown that G is induction equivalent to G_{k-1} , where G_{k-1} has no symbols S_2, \ldots, S_{k-1} .

Then start by detaching all edges labelled with symbols S_{k+2}, \ldots, S_m . Call the resulting tree \widetilde{G} . By [CFZ10, 5.2] there is a sequence of inductions of the form $R_{1,k}$ and $L_{k,k+1}$ taking \widetilde{G} to \widetilde{G}_k , where \widetilde{G}_k has no edges labelled S_2, \ldots, S_k . Reattach the detached edges and call the resulting tree G_k . Since none of the reattached edges are labelled by S_1, S_k , or S_{k+1} , this sequence of inductions takes G_{k-1} to G_k by identifying the maximal chains in \widetilde{G} with the maximal chains in G_{k-1} . Note that none of the symbols S_2, \ldots, S_k appears in G_k . Hence, by induction on k, we can construct $G_{m-1} = G_*$ with no symbols S_2, \ldots, S_{m-1} and a sequence of inductions, each of form R_{ij} (with $j \leq m-1$) or L_{ij} (with $i \geq 2$) taking G to G_* .

Remark 6.6. In the above proof, the inductions $R_{1,k}$ are applied in a situation satisfying the hypotheses of Lemma 6.2, and hence each can be written as a product of the inductions R_1, \ldots, R_{k-1} .

Corollary 6.7. Let G be a tree of relations. There exists a tree of relations G_* containing only symbols S_1 and S_m and a sequence of inductions, each of the form R_i or L_i , taking G to G_* .

Corollary 6.8. Let G be a connected tree of relations with k vertices. Then every possible connected shape with k vertices appears as the shape of a tree of relations in $\Gamma(G)$.

Proof. Let S and S' be arbitrary connected shapes. Then, by Corollary 6.7, S is induction equivalent to a shape containing only the symbols S_1 and S_m ; similarly for S' (see Remark 6.3(3)). If k is odd there is only one such shape:

$$\cdot \ \ \, \underbrace{S_m \quad \cdot \quad S_1 \quad \cdot \quad S_m} \quad \cdot \quad \dots \quad \cdot \quad \underbrace{S_1 \quad \cdot \quad \cdot \quad }_{S_1} \quad \cdot \quad \cdot \quad \dots$$

and it follows that S and S' are inductively equivalent. If k is even, there are two shapes with symbols S_1 and S_m :

$$S_m: \cdot \xrightarrow{S_m} \cdot \xrightarrow{S_1} \cdot \xrightarrow{S_m} \cdot \cdots \cdot \xrightarrow{S_m} \cdot S_1: \cdot \xrightarrow{S_1} \cdot \xrightarrow{S_m} \cdot \xrightarrow{S_1} \cdot \cdots \cdot \xrightarrow{S_1} \cdot \cdots$$

Then $R_{1,\hat{m}}^{S_m}(S_m) = S_1$, so S_m is induction equivalent to S_1 by Lemma 6.2. It follows that S and S' are induction equivalent in this case also.

Given a connected tree of relations, G of shape S, and an arbitrary connected shape, S', the above shows that S and S' are inductively equivalent. It follows that G and a filling of S' are inductively equivalent, and the result follows.

Remark 6.9. It follows from the above proof that every possible shape with k vertices appears as the shape of a tree of relations in $\Gamma_{Gen}(G)$.

Corollary 6.10. If there is a sequence of general inductions of the form $R_{i,j}$ and $L_{i,j}$ between two shapes then they are induction equivalent (i.e. equivalent under L_i and R_i induction).

Proof. This follows immediately from Corollary 6.8, since in fact any two shapes are induction equivalent. \Box

We shall see below that the corresponding result does not hold for trees of relations (see Remark 6.15).

- **Lemma 6.11.** (a) Let k be odd, let $i \neq j$ and let G be a tree of relations with k vertices and whose edges are decorated with symbols S_i and S_j only. Let S be the shape of G. Applying $R_{i,j}$ induction on G has order k, producing k distinct trees with shape S.
- (b) Let k be even, $i \neq j$ and let G be a tree of relations with k vertices and whose edges are decorated with symbols S_i and S_j only. Let S be the shape of G. Applying $R_{i,j}$ induction to G has order k, producing k/2 trees of relations of shape S and k/2 trees of relations of shape $R_{i,j}(S)$.
- *Proof.* (a) Since S only contains the symbols S_i and S_j , it is a line. Suppose the line is drawn horizontally and suppose the leftmost edge has label S_j and vertices a_1 and a_2 from left to right. Then in $R_{i,j}^d(G)$, if it is drawn with orientation given
- by $\cdot \frac{S_i}{dt} = a_1 \frac{S_j}{dt}$ (where one of the edges may not exist), the vertex a_1 is the d^{th} vertex from the left. It is clear that all the induced trees $R^d_{i,j}(G)$ have the same shape (those for d odd should be read from right to left).
- (b) The proof is similar to the one in (a), except that for d odd, the shape of $(R_{i,j}(G))^d$ is $R_{i,j}(S)$.

Remark 6.12. (1) Since in the context of Lemma 6.11 the shape of G is a line, we can replace $R_{i,j}$ in Lemma 6.11 by $R_i \dots R_{j-2}R_{j-1}R_{j-2}\dots R_i$.

- (2) If we replace the R induction in Lemma 6.11 by L induction, the result holds and is proved by a similar argument.
- **Lemma 6.13.** Let G be a tree of relations containing a maximal S_i - S_j chain B with no incident edges labelled S_k , i < k < j. Then the circular order, σ_G , is unchanged after $R_{i,j}$ or $L_{i,j}$ induction on B is applied.

Proof. We show that the circular order is invariant under R_{ij} -induction in the context given (the proof for $L_{i,j}$ -induction follows a similar argument).

Let G be a tree of relations with circular order σ_G and containing a maximal S_i - S_j -chain B and such that no edges labelled S_k , for i < k < j are incident to B. Let $G' = R_{i,j}^B(G)$ with circular order $\sigma_{G'}$. Let i < j and let a be a vertex in B. Let S'_1, \ldots, S'_m denote the maps corresponding to the symbols S_1, \ldots, S_m in the tree of relations G'. Then we have, similarly to [CFZ10, 3.6], that $S_jS_iS_j(a) = S'_j(a)$, $S_j(a) = S'_i(a)$ and, for $k \neq j$, $S_k(a) = S'_k(a)$. Similarly, after applying $L_{i,j}$ -induction, we have $S_iS_jS_i(a) = S'_i(a)$, $S_i(a) = S'_j(a)$ and, for $k \neq i$, $S_k(a) = S'_k(a)$. There are three possible situations to consider.

Case 1: Suppose first that a has an incident edge labelled with symbol S_k with $1 \le k < i$. We assume that k is minimal. Let T be the subtree of $G \setminus B$ connected to a via this edge. Then $\sigma_G(a)$ lies in T. Applying the induction $R_{i,j}^B$ to G results in a tree of relations G' in which a is reconnected to T by the edge labelled with symbol S_k . Therefore $\sigma_G(a) = \sigma_{G'}(a)$.

Case 2: Suppose that a is not incident with any edges labelled with symbols S_k for k < i, but that the tre vertex $S_j S_i(a)$ has an incident edge labelled with symbol S_k where $j < k \le m$. We take k minimal. Let T be the subtree of $G \setminus B$ connected to $S_j S_i(a)$ via this edge. Then $\sigma_G(a)$ lies on the subtree T. Applying $R_{i,j}^B(G)$ results in a tree of relations G' such T is reconnected, via the edge labelled S_k , to $S_j' S_i'(a) = S_j S_i(a)$. Therefore $\sigma_G(a) = \sigma_{G'}(a)$.

Case 3: Suppose that neither a nor $S_jS_i(a)$ has any incident edges labelled S_k , for $k \neq i, j$. Then $S_k(a) = a$ for all $k \neq i, j$ and $S_k(S_jS_i(a)) = S_jS_i(a)$ for all $k \neq i, j$. By our assumptions, for i < k < j, we have that $S'_k = S_k$ on the whole maximal chain. Hence, using the relations from the beginning of the proof,

$$\sigma_{G'}(a) = S'_m \cdots S'_1(a)$$

$$= S'_m \cdots S'_{j+1} S'_j S'_i(a)$$

$$= S'_m \cdots S'_{j+1} S_j S_i(a)$$

$$= S_j S_i(a)$$

$$= S_m \cdots S_{j+1} S_j S_i(a)$$

$$= S_m \cdots S_1(a).$$

Corollary 6.14. The circular order of a tree of relations is invariant under R_i and L_i induction.

Proof. In Lemma 6.13 assume that j = i + 1.

Remark 6.15. In general, the circular order of a tree of relations is not invariant under general $R_{i,j}$ and $L_{i,j}$ induction for i < j+1: in the above proof suppose that we have an edge S_k , for i < k < j connected to $S_i(a)$ in the maximal chain B of G and let T be a subtree of G connected to S_k . Then $\sigma_G(a)$ lies on the subtree T. On the other hand in $R_{i,j}^B(G)$, the edge S_k is connected to $S_i(a) = S_i'S_j'S_i'(a)$ and thus $\sigma_{G'}(a) \neq \sigma_G(a)$ in general. For an example of this with i = 1 and j = 3 (and T just consisting of one vertex), see Figure 8.

Note that this means that it is not possible, in general, to write R_{ij} as a composition of inductions of form R_i and L_i , despite Lemma 6.2 (which says that sometimes this is possible).

We finally achieve the generalisation of [CFZ10, 6.2] that we were aiming for:

Theorem 6.16. Let G and G' be trees of relations. Then G' is in $\Gamma(G)$ if and only if $\sigma_G = \sigma_{G'}$.

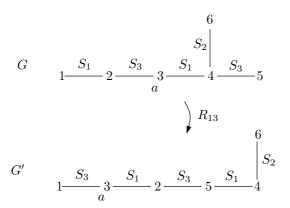


FIGURE 8. R_{13} -induction does not preserve the circular order: $\sigma_G(3) = 6$ while $\sigma_{G'}(3) = 5$

Proof. Suppose that G' is in $\Gamma(G)$. It then follows directly from Lemma 6.14 that $\sigma_G = \sigma_{G'}$. Conversely, suppose that $\sigma_G = \sigma_{G'}$. By Corollary 6.7 and the proof of Corollary 6.8 there exist trees of relations G_* in $\Gamma(G)$ and G'_* in $\Gamma(G')$ where the shape of G_* and the shape of G'_* contains symbols S_1 and S_m only.

Suppose that k is odd and that G_* and G'_* are as follows:

$$G_*: a_1 \xrightarrow{S_i} a_2 \xrightarrow{S_j} a_3 \xrightarrow{S_i} a_4 \qquad \cdots \qquad a_{r-1} \xrightarrow{S_j} a_k$$

 $G'_*: a'_1 \xrightarrow{S_i} a'_2 \xrightarrow{S_j} a'_3 \xrightarrow{S_i} a'_4 \qquad \cdots \qquad a'_{r-1} \xrightarrow{S_j} a'_k$

Then $\sigma_{G_*} = (a_1 a_2 a_4 \dots a_{k-1} a_k a_{k-2} \dots a_3) = (a'_1 a'_2 a'_4 \dots a'_{k-1} a'_k a'_{k-2} \dots a'_3) = \sigma_{G'_*}$. Because of its shape, G'_* is determined by a'_1 and its circular order. Thus, given G_* there are at most k possibilities for G'_* such that $\sigma_{G_*} = \sigma_{G'_*}$ holds.

By Lemma 6.11, Remark 6.12, and Lemma 6.14, repeatedly applying either $R_{i,j}$ -induction or $L_{i,j}$ -induction to G_* gives k distinct trees of relations H satisfying $\sigma_{G_*} = \sigma_H$. Hence any G'_* such that $\sigma_{G_*} = \sigma_{G'_*}$ must be one of these trees H. Therefore G'_* is in $\Gamma(G_*)$ and thus G' is in $\Gamma(G)$.

Suppose that k is even. In this case, there are at most k/2 distinct possibilities for G'_* because of the symmetry of the shape. The result then follows from Lemma 6.11, Remark 6.12, and Lemma 6.14 as above.

7. Induction on m-Angulations of Polygons

As we have seen in section 2, trees of relations with k vertices and m symbols are in bijection with m-gon-labelled diagonal-labelled m-angulations of polygons (recall that m-gon-labelled means that the m-gons in the m-angulation are labelled with the numbers $1,2,\ldots,k$). Such polygons have n=(m-2)k+2 sides. The edge labels of the m-angulations correspond to the symbols S_1,\ldots,S_m in a clockwise order around each m-gon. Similarly, shapes with k vertices are in bijection with diagonal-labelled m-angulations of polygons with k m-gons.

Our aim in this section is to rewrite induction in the language of (m-2)-clusters. We saw in Theorem 3.1 that m-angulations of a polygon containing k m-gons are in bijection with (m-2)-clusters in the sense of Fomin-Reading [FR05] of type A_{k-1} . For such clusters, mutation corresponds to rotating a diagonal one step anticlockwise in the subpolygon with 2m-2 sides obtained when the diagonal is removed. We shall see that induction has an interesting description as a composition of such mutations (which we shall refer to as anticlockwise diagonal rotations): see Proposition 7.5, below.

Lemma 7.1. Every m-angulation \mathcal{M} of a polygon has at least two m-gons with m-1 boundary edges or is an m-angulation of an m-gon.

Proof. The result is clearly true if \mathcal{M} is an m-angulation of an m-gon. Let \mathcal{M} be an m-angulation of P_n , and assume that all m-angulations of polygons with fewer sides have two boundary m-gons or are just one m-gon. Cutting \mathcal{M} along one of its m-diagonals D gives two m-angulations of polygons with fewer sides. By the induction hypothesis, each of these polygons contains an m-gon incident with its boundary and the result follows.

In the following two lemmas we describe how to use anticlockwise rotations of diagonals to rotate an m-angulation of an n-gon (containing k m-gons) anticlockwise through $2\pi/n$. Note that any clockwise rotation can easily be achieved via a composition of anticlockwise rotations; we shall therefore sometimes use clockwise rotations. We use the notation [i,j] to describe a diagonal in the polygon connecting vertex i with vertex j.

Lemma 7.2. Let P_n be an n-gon with vertices labelled 1 through n. Suppose P_n has an m-angulation \mathcal{M} by k m-gons with diagonals $[1, m], [1, m + (m-2)], [1, m + 2(m-2)], \ldots, [1, m+(k-2)(m-2)]$. Then there is an explicit sequence of diagonal rotations taking \mathcal{M} to its rotation through $2\pi/n$ anticlockwise.

Proof. We apply the following anticlockwise diagonal rotations:

$$\begin{array}{lll} [1,m+(k-2)(m-2)] & \to & [n,m+(k-2)(m-2)-1] \\ [1,m+(k-3)(m-2)] & \to & [n,m+(k-3)(m-2)-1] \\ \vdots & & \vdots & \vdots \\ [1,m+r(m-2)] & \to & [n,m+r(m-2)-1] \\ \vdots & & \vdots & \vdots \\ [1,m] & \to & [n,m-1] \end{array}$$

This produces an m-angulation \mathcal{M}' of P_n with diagonals $[n, m + (k-2)(m-2)-1], [n, m+(k-3)(m-2)-1], \ldots, [n, m+r(m-2)-1], \ldots, [n, m-1]$ which corresponds to an anticlockwise rotation of \mathcal{M} through $2\pi/n$.

Lemma 7.3. Let \mathcal{M} be an m-angulation of P_n containing k m-gons. Then there is an explicit sequence of diagonal rotations taking \mathcal{M} to its rotation through $2\pi/n$ anticlockwise.

Proof. Suppose P_n has an m-angulation \mathcal{M} by k m-gons. Let M be an m-gon with m-1 boundary edges and one internal edge e joining vertices [i,i+(m-1)]. Let R be the union of the m-gons incident with i. Apply Lemma 7.2 to the induced m-angulation of R to rotate it one step anticlockwise. Let R' be the subpolygon R with the m-gon M' with vertices $i-1,i,i+1,\ldots,i+(m-1)-1$ removed. Apply the reverse sequence to the one described in Lemma 7.2 to rotate the m-angulation of R' one step clockwise (recalling that a clockwise rotation of a diagonal coincides with a composition of anticlockwise rotations of the same diagonal). Consider the polygon Q which is given by removing the m-gon M' from P_n and transform it (using an orientation-preserving homeomorphism) to a regular n-(m-2)-gon $P_{n-(m-2)}$. Since $P_{n-(m-2)}$ has fewer sides than P_n we have inductively constructed a sequence of anticlockwise diagonal rotations rotating the m-angulation of $P_{n-(m-1)}$ anticlockwise through $2\pi/(n-(m-1))$. Applying the corresponding sequence to the m-angulation of Q takes \mathcal{M} to its rotation anticlockwise through $2\pi/n$ as required.

Definition 7.4. Let \mathcal{M} be an m-angulation of P_n , diagonal-labelled with symbols S_1, S_2, \ldots, S_m . If there is at least one internal diagonal in \mathcal{M} and all of the internal diagonals of \mathcal{M} are labelled only with symbols S_i or S_j for fixed i, j, we call \mathcal{M} a snake m-angulation. A subpolygon of P_n with this property is called a snake subpolygon. Note that in any snake subpolygon the internal diagonals must be of the form $[i_1, i_2], [i_2, i_3]$, and so on, and the internal angle between diagonals $[i_{r-1}, i_r]$ and $[i_r, i_{r+1}]$ must alternate between being positive and negative as r increases.

We note that such snake m-angulations first appeared in the context of cluster algebras in Fomin-Zelevinsky's article [FZ03] (for the case m=3, i.e. triangulations) and appeared for general m in [FR05] under the name m-snake. We now show how they can be used to describe R_i induction as a sequence of (m-2)-cluster mutations, i.e. anticlockwise diagonal rotations.

Proposition 7.5. Let \mathcal{M} be an m-angulation of P_n such that the edges of all m-gons of P_n are labelled by symbols S_1, \ldots, S_m in a clockwise order. Then R_i induction on P_n can be described in terms of a sequence of anticlockwise diagonal rotations.

Proof. Choose a maximal snake subpolygon with internal diagonals labelled S_i or S_{i+1} . Then R_i -induction on B is given as follows.

Step 1: It is easy to see that the induced m-angulation of B contains exactly two m-gons with m-1 boundary edges in B.

We fix M_1 to be one such m-gon M. Let M_2 be the unique m-gon adjacent to M_1 , M_3 the unique m-gon adjacent to M_2 , and so on, with M_l the unique m-gon in B adjacent to M_{l-1} for each l.

If e_{M_1} has label S_i , rotate the diagonal between M_2 and M_3 one step anticlockwise, then rotate the diagonal between M_4 and M_5 one step anticlockwise and continue like this until there are 0 or 1 m-gons left in B.

If e_M is labelled S_{i+1} , rotate the diagonals between M_1 and M_2 , M_3 and M_4 , etc. one step anticlockwise until there are 0 or 1 m-gons left in B.

Exchange the labels of the edges with labels S_i and S_{i+1} in B and relabel the boundary edges in B as required (using the rule that each m-gon in B must have the symbols S_1, S_2, \ldots, S_m clockwise on its boundary).

Step 2: For each connected component C of the complement of B in P_n incident with an m-gon M inside B with m-1 boundary edges in B and with internal edge labelled by S_i , let $D = C \cup M$. Apply Lemma 7.3 to D to get a sequence of anticlockwise rotations rotating the induced m-angulation of D anticlockwise. Should no such C exist, no action is necessary.

- **Remark 7.6.** (1) Step 2 in the above proof has the same effect as detaching C from M and reattaching C with the same edge to a boundary edge of M one step anticlockwise around the boundary of M.
 - (2) For L_i induction replace all anticlockwise rotations by clockwise rotations and vice versa.

Finally in this section, we show how the above can be modified in the case where the m-gons are labelled; at the same time we reduce the number of anticlockwise diagonal rotations required by allowing detaching and reattaching of subpolygons.

Proposition 7.7. Let \mathcal{M} be a diagonal-labelled m-angulation of an n-gon P_n by k labelled m-gons, where the edges of the m-gons are labelled by the symbols $S_1, \ldots S_m$ in a clockwise order and the m-gons are labelled $1, \ldots, k$. Then R_i induction on P_n can be described in terms of detaching and reattaching subpolygons and a sequence of anticlockwise diagonal rotations.

Proof. We start with a diagonal-labelled, m-gon labelled m-angulation \mathcal{M} of P_n into k m-gons. We describe the procedure of R_i induction on some maximal snake subpolygon B of \mathcal{M} with r edges with labels on internal edges S_i and S_{i+1} .

Detach all subpolygons in the complement of B in P_n . We know that the m-angulation of B has exactly two m-gons with m-1 boundary edges in B. Let M_1 be one of them with internal edge e. Let M_2 be the unique m-gon adjacent to M_1 , M_3 the unique m-gon adjacent to M_2 , and so on.

If e is labelled S_i , rotate the diagonal between M_2 and M_3 one step anticlockwise. Let M'_2 and M'_3 be the new m-gons created, with M'_3 adjacent to M_1 . Repeat for M_4 and M_5 , M_6 and M_7 , etc until 0 or 1 m-gons are left.

If e is labelled S_{i+1} , rotate the diagonal between M_1 and M_2 one step anticlockwise; call the new m-gons created M'_1 and M'_2 with M'_2 incident with a bouldary edge of M_1 . Repeat for M_3 and M_4 , etc. until 0 or 1 m-gons are left.

Relabel all edges in B, starting by exchanging labels S_i and S_{i+1} on the diagonals of B and then using the rule that every m-gon inside B must have the symbols S_1, \ldots, S_m clockwise on its boundary. Reattach each detached subpolygon to the m-gon with the same label it was originally attached to via the edge with the same symbol. The new m-gon label of M'_i is defined to be the old m-gon label of M_i . \square

Remark 7.8. It is easy to see that neither induction procedure described above depends on the initial choice of M as m-gon of B with m-1 boundary edges.

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