POSETS AND SPACES OF K-NONCROSSING RNA STRUCTURES *

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Abstract. RNA molecules are single-stranded analogues of DNA that can fold into various structures which influence their biological function within the cell. RNA structures can be modelled combinatorially in terms of a certain type of graph called an RNA diagram. In this paper we introduce a new poset of RNA diagrams $\mathcal{B}^r_{f,k}$, $r \geq 0$, $k \geq 1$ and $f \geq 3$, which we call the Penner-Waterman poset, and, using results from the theory of multitriangulations, we show that this is a pure poset of rank $k(2f-2k+1)+r-f-1$, whose geometric realization is the join of a simplicial sphere of dimension $k(f-2k)-1$ and an $((f+1)(k-1)-1)$-simplex in case $r=0$. As a corollary for the special case $k=1$, we obtain a result due to Penner and Waterman concerning the topology of the space of RNA secondary structures. These results could eventually lead to new ways to study landscapes of RNA k-noncrossing structures.

Key words. RNA structures, k-noncrossing pseudoknots, Multitriangulations, Poset topology

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1. Introduction. Ribonucleic acid (RNA) is a single-stranded polymeric molecule that is essential in various biochemical processes within the cell. The primary structure of an RNA molecule is a linear sequence of four nucleotides, also known as *bases* and usually denoted by A (adenine), C (cytosine), G (guanine) and U (uracil). In nature, RNA molecules fold into structures which are intimately related to their biological function. These structures arise from the linear sequence folding back onto itself which is possible since the non-adjacent bases A/U and G/C can form bonds or *base-pairs*. Motivated by this phenomenon, there has been a great deal of interest in the prediction of RNA structures [6], and also in understanding combinatorial properties of these structures over the past three decades [3, 8, 13, 17, 19].

RNA structures are commonly represented by *binary diagrams*, simple graphs drawn in the plane in which each base is represented by a vertex and the underlying linear molecule is represented by a collection of edges along a horizontal line. In addition, the base-pairs are represented by semi-circles or *arcs* in the upper halfplane such that arcs do not connect the last and first bases and no two arcs are incident with the same vertex (see e.g. Fig. 1(i)). In the special case where the diagram representing an RNA structure has no intersecting arcs, the RNA structure is also known as a *secondary structure*. RNA secondary structures are important as they often form a backbone structure for an RNA molecule, and their nested structure facilitates their prediction using free-energy models [6, pp. 1-31].

In [13] Penner and Waterman introduce and study a certain *space* of RNA secondary structures. In combinatorial language, this space can be considered as the geometric realization of a certain finite poset $\mathcal{B}^r_f$ of RNA secondary structures for $r \geq 0$ and $f \geq 3$ whose definition we now recall. We call a base in a diagram a *free site* if it is not contained in any arc, and an arc e *tautological* if either e covers precisely one free site or there exists an arc below e that covers the same set of free sites as e. The poset $\mathcal{B}^r_f$ then consists of all RNA secondary structures whose diagrams have f free sites and no more than r tautological arcs. For example, the RNA secondary structure in Fig. 1(i) is in $\mathcal{B}^2_3$. The poset relation on $\mathcal{B}^r_f$ is induced by *arc suppression*,

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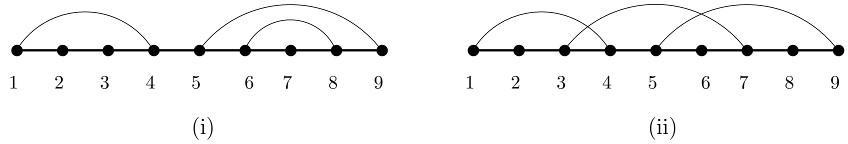


Fig. 1: (i) An RNA secondary structure with 9 bases (represented by black vertices) and 3 base-pairs (represented by arcs). In this diagram, the arc $(1, 4)$ covers free sites 2 and 3, and the arc (6,8) is below the arc (5,9). (ii) An RNA pseudoknot that is a 2-noncrossing structure with 3 base-pairs.

that is, removal of an arc and the two sites which it contains from a diagram (for the formal definition see Section 2.1). In Fig. 2(i) we present the Hasse diagram of the poset $\mathcal{B}_4^0$.

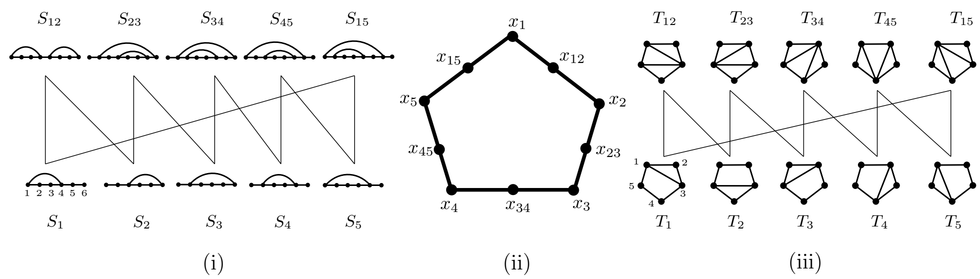


Fig. 2: (i) The Hasse diagram of the poset $\mathcal{B}_4^0$. (ii) The geometric realization of the poset $\mathcal{B}_4^0$. Here the vertices x_i and x_{ij} correspond to RNA secondary structures S_i, S_{ij} with the same indices. (iii) The Hasse diagram of the poset $\mathcal{T}_5$, whose elements are the triangulations of a pentagon. The poset isomorphism between $\mathcal{B}_4^0$ and $\mathcal{T}_5$ mentioned in the text maps each secondary structure in $\mathcal{B}_4^0$ to the triangulation in $\mathcal{T}_5$ with the same indices.

Penner and Waterman show that the poset $\mathcal{B}_f^0$ is isomorphic to what they call the *arc poset* $\mathcal{T}_{f+1}$ on a $(f+1)$-gon [13, Proposition 3], whose elements can be considered as the set of triangulations of a $(f+1)$-gon. This enables them to then show that the geometric realization of the poset $\mathcal{B}_f^0$ is a topological sphere of dimension $f-3$. For example, in Fig. 2(iii) the poset $\mathcal{T}_5$ is pictured together with the geometrical realization of the poset $\mathcal{B}_4^0$, which is the simplicial complex consisting of ten 1-simplices as pictured in Fig. 2 (ii). This complex is clearly homeomorphic to a 1-dimensional sphere.

1.1. The Penner-Waterman poset. By definition, diagrams corresponding to structures in the poset $\mathcal{B}_f^r$ contain no arcs that pairwise intersect. However, RNA molecules can fold into structures whose corresponding diagrams contain pairs of crossing arcs. In this case, the RNA structure is no longer a secondary structure but what is commonly called an RNA *pseudoknot*. RNA pseudoknots are wide-spread in nature and have important functions [3]. We are therefore interested in how to extend Penner and Waterman's analysis to these more complicated structures.

To this end, we focus on a special type of pseudoknot called a *k-noncrossing structure* (see, e.g. [8]). This is an RNA structure whose diagram does not contain $(k+1)$ arcs that are pairwise mutually crossing. See Fig. 1(ii) for an example of 2-noncrossing pseudoknot; among the three arcs in the pseudoknot, only arcs $(1,4)$ and $(5,9)$ do not form a crossing pair. Note that k-noncrossing structures are also called $(k+1)$-noncrossing structures by some authors (e.g. [8]). RNA k-noncrossing structures have been studied extensively in the past decade (see, e.g. [3], and the reference therein), and they have interesting combinatorial properties (see, e.g. [17]).

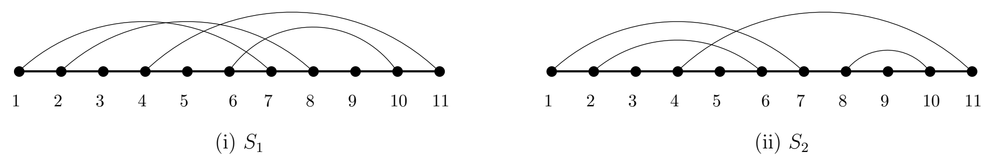


Fig. 3: (i) A 3-noncrossing diagram S_1 in $\mathcal{P}^2_{3,3}$, which is not regular as $(1,7)$ and $(2,8)$ are two mutually crossing arcs both incident with the interval consisting of the non-free sites 1 and 2. (ii) A 2-noncrossing diagram S_2 in $\mathcal{B}^2_{3,2}$ which is regular and equivalent to S_1.

In this paper, we define and study a new poset $\mathcal{B}^r_{f,k}$ ($k \geq 1$, $f \geq 3$, $r \geq 0$) of binary RNA k-noncrossing structures whose diagrams are *regular* and which contain exactly f free sites and have tautological number at most r. Intuitively, a regular diagram is one in which there are no two crossing arcs that are both incident with the same interval of non-free sites (see Fig. 3(ii) for an example and Section 3 for the precise definition). We call the poset $\mathcal{B}^r_{f,k}$ the *Penner-Waterman poset* since, as we shall see later, $\mathcal{B}^r_{f,1} = \mathcal{B}^r_f$.

The two main results of this paper concern the Penner-Waterman poset. The first gives the structure of the geometric realization of $\mathcal{B}^0_{f,k}$ (see Section 2 for the definition of this term).

Theorem 1.1. *For two integers $k \geq 1$ and $f \geq 3$ with $f \geq 2k$, the geometric realization of $\mathcal{B}^0_{f,k}$ is the join of a simplicial sphere of dimension $k(f-2k)-1$ and an $((f+1)(k-1)-1)$-simplex.*

An illustration of Theorem 1.1 is presented in Fig. 4 for a subposet of $\mathcal{B}^0_{5,2}$ (the full poset is too large to include). Our second main result concerns the structure of $\mathcal{B}^r_{f,k}$. Recall that rank of a (finite) poset is the length of a maximum length in the poset, and that the poset is pure in case all of its maximal chains have the same length.

Theorem 1.2. *For any $r \geq 0$, $f \geq 3$ and $k \geq 1$ with $f \geq 2k$, the Penner-Waterman poset $\mathcal{B}^r_{f,k}$ is pure and of rank $k(2f-2k+1)+r-f-1$.*

As a corollary, we also obtain an independent proof of Penner and Waterman's result mentioned above concerning the topology of $\mathcal{B}^0_f$.

1.2. Outline of the proof of Theorems 1.1 and 1.2. As the proof of our main results is quite technical and involved (see Section 8), we now provide an overview to guide the reader through it. Our main tool is the introduction of an algebraic relationship which associates a certain type of symmetric integral matrix to k-noncrossing structure which we call its *block matrix*. Intuitively, these matrices encode the inci-

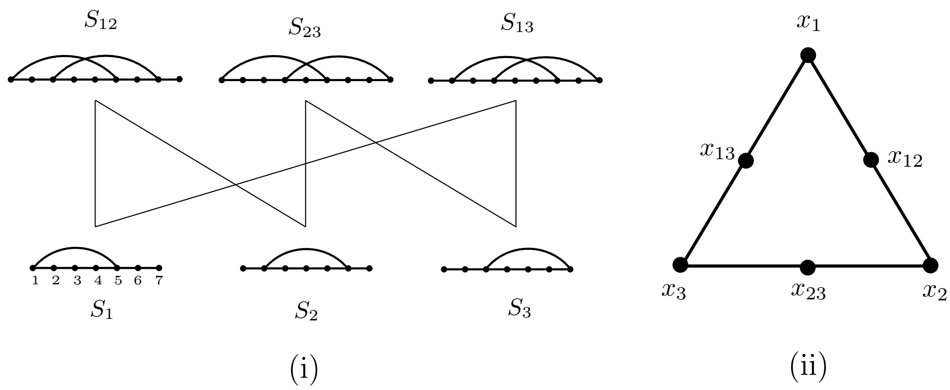


Fig. 4: (i) The Hasse diagram of a subposet of $\mathcal{B}^0_{5,2}$. (ii) The geometric realization of the subposet in (i), which is a simplicial sphere of dimension one. Here the vertices x_i and x_{ij} correspond to RNA secondary structures S_i, S_{ij} with the same indices.

dence relationship between blocks of an RNA structure, where a block is a maximal interval of non-free sites. For instance, in the diagram S_1 in Fig. 3 the interval consisting the of non-free sites 6, 7, and 8 is a block; there are two arcs between this block and the block consisting of the non-free sites 1 and 2, which is encoded as an entry with value 2 in the associated block matrix. We took this approach since Penner and Waterman used *rooted fattrees* to prove their results but, even though fattrees can be generalized to fatgraphs (see e.g [14]), we could not find a way to utilize this generalization in our proofs.

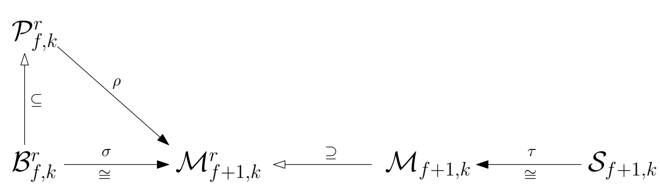


Fig. 5: An outline of the proof of the main results. Here $\mathcal{P}^r_{f,k}$ is the poset of proper k-noncrossing diagrams with f free sites whose tautology number is at most r. The Penner-Waterman poset $\mathcal{B}^r_{f,k}$ contains all regular diagrams in $\mathcal{P}^r_{f,k}$, and $\mathcal{M}^r_{f+1,k}$ is the poset consisting of the block matrices of the diagrams in $\mathcal{B}^r_{f,k}$, which are certain non-negative integral k-noncrossing matrices of order $f+1$. Next, $\mathcal{S}_{f+1,k}$ is the poset of all (not necessarily binary) k-noncrossing diagrams with $f+1$ free sites. Among the three poset homomorphisms, ρ is surjective whilst both σ and τ are isomorphisms.

Our proof proceeds as follows (see Fig. 5). The first goal is to show that $\mathcal{B}^r_{f,k}$ is isomorphic to the poset $\mathcal{M}^r_{f+1,k}$ of a certain family of symmetric integral matrices of order $f+1$ (Theorem 7.1). To this end, we introduce the set $\mathcal{P}^r_{f,k}$ of *proper* diagrams, a superset of $\mathcal{B}^r_{f,k}$ consisting of binary diagrams in which each arc covers at least one, but not all of the free sites in the diagram (see Fig. 3 for an example), and consider the map ρ which takes each diagram in $\mathcal{P}^r_{f,k}$ to its block matrix. To show that ρ is surjective, we begin by defining an equivalence relation $\sim$ on $\mathcal{P}^r_{f,k}$, where $S \sim S'$ holds for two proper diagrams S and S' if and only if there exists a bijection between the arcs of S to those of S' that preserves the free sites below each arc. We then show that two proper diagrams are equivalent if and only if they have the same block matrix (Theorem 5.5), and that there exists a unique regular diagram within each equivalence class of $\sim$, namely the diagram with the minimum number of crossing arc pairs among all proper diagrams within that class (Theorem 6.4). Using a characterisation of integral matrices that can be realized as the block matrix of a proper diagram (Theorem 7.3), we then show that the collection of preimages $\{\rho^{-1}(\mathbf{M}) : \mathbf{M} \in \mathcal{M}^r_{f+1,k}\}$ forms a partition of $\mathcal{P}^r_{f,k}$, and that each preimage is precisely one of the equivalence classes of $\sim$. From this it follows that ρ is surjective and, moreover, that its restriction to $\mathcal{B}^r_{f,k}$, denoted by σ, is a poset isomorphism between $\mathcal{B}^r_{f,k}$ and $\mathcal{M}^r_{f+1,k}$ (Theorem 7.1).

Our second goal is to show that $\mathcal{B}^0_{f,k}$ is isomorphic to $\mathcal{S}_{f+1,k}$, the poset of all (not necessarily binary) k-noncrossing diagrams with $f+1$ free sites (Theorem 7.4). To do this, we show that mapping a diagram in $\mathcal{S}_{f+1,k}$ to its adjacency matrix gives a poset isomorphism τ from $\mathcal{S}_{f+1,k}$ to $\mathcal{M}^0_{f+1,k}$ (Proposition 2.1). Composing σ with the inverse of the map τ in case $r = 0$ then gives a poset isomorphism between $\mathcal{B}^0_{f,k}$ and $\mathcal{S}_{f+1,k}$.

The proof of our main results is then completed by exploiting an interesting connection between $\mathcal{S}_{f+1,k}$ and a certain poset of *multitriangulations* of a polygon [15], as detailed in Lemma 8.2. Since the topology of the poset of multitriangulations is well understood, this enables us to obtain the topology of $\mathcal{B}^0_{f,k}$ in Theorem 1.1 and, as a corollary, the fact that $\mathcal{B}^r_{f,k}$ is pure in Theorem 1.2.

1.3. Organization of the rest of the paper. In Section 2 we collect together some basic terminology and facts concerning diagrams and simplicial complexes. We then introduce block matrices and regular diagrams in Section 3, and the Penner-Waterman poset and $\mathcal{M}^r_{f+1,k}$ in Section 4. In Section 5 we define the equivalence relation $\sim$ on proper diagrams, and in Section 6 we show that there exists a unique regular diagram within each equivalence class of $\sim$. In Section 7 we show that the map σ is a poset isomorphism between the Penner-Waterman poset $\mathcal{B}^r_{f,k}$ and the poset $\mathcal{M}^r_{f+1,k}$, and that $\tau^{-1}\sigma$ gives a poset isomorphism between $\mathcal{B}^0_{f,k}$ and $\mathcal{S}_{f+1,k}$. Then in Section 8 we prove our main results by considering the above-mentioned relationship between $\mathcal{S}_{f+1,k}$ and multitriangulations. In the last section, we conclude with a brief discussion of some possible future directions.

2. Preliminaries.

2.1. Diagrams. In this paper, n and k are two positive integers with $n \geq 4$ and $k \geq 1$, unless stated otherwise.

Motivated by [7, 13], a *molecule diagram*, or just *diagram*, is a graph with vertex set $\{1, \dots, n\}$, where each vertex is called a *site*. It consists of *base-pair* arcs, which are of the form (s_1, s_2) with $1 < s_2 - s_1 < n - 1$, as well as $n - 1$ backbone edges which are of the form $\{i, i+1\}$ for $1 \leq i \leq n-1$. In particular, the arc $(1, n)$ is not allowed in any diagram. Note that the backbone edges play no part in our results, but we include them as it is usual to do so in the definition of RNA secondary structures. In particular, from now on all arcs that we consider will be base-pair arcs. In figures of diagrams backbone edges are represented by horizontal lines, and base-pairs by semi-circles in the upper-half plane (see Fig. 6 for an example). The *length* and *size* of a diagram are the number of vertices and arcs, respectively. A diagram is *trivial* if its size is zero, and *non-trivial* otherwise.

Two sites s and s' are *adjacent* if $|s - s'| = 1$ holds, and when $s < s'$, we denote the *interval* that contains all sites between s and s' by $[s, s']$. In case (s_1, s_2) is an arc we say that s_1 and s_2 are *base-paired*, and that (s_1, s_2) is *supported* by s_1 and s_2. Two arcs are *adjacent* if one of them is supported by a site s and the other by a site adjacent to s. A site s is called *free* if it does not support any arc, and it is *covered* by an arc (s_1, s_2) if $s_1 < s < s_2$ holds. An arc is called *degenerate* if it does not cover any free site, and *tiny* if it covers precisely one free site.

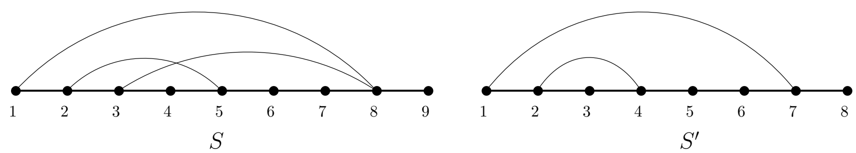


Fig. 6: Two RNA diagrams: S is 2-noncrossing with length 9 and size 3, and S' is binary 1-noncrossing. Note that S' is obtained from S by suppressing the arc $(3, 8)$.

A diagram S is called *binary* if it is non-trivial and each site supports at most one arc, and it is called *proper* if it is binary and each arc covers at least one free site but no arc covers all of the free sites in S. Note that a proper diagram has a length of at least four and contains at least two free sites. Two arcs (s_1, s_2) and (s'_1, s'_2) in a diagram are *crossing* if either $s_1 < s'_1 < s_2 < s'_2$ or $s'_1 < s_1 < s'_2 < s_2$ holds. A diagram is a *k-noncrossing diagram* if it does not contain $(k+1)$ mutually crossing arcs, $k \geq 1$. Note that binary 1-noncrossing diagrams are the RNA secondary structures defined in the introduction (see e.g. [13]). Also, the parameter k in the definition of a k-noncrossing diagram is used in a way similar to that in a k-triangulation (see Section 8 and, e.g. [21]). While some authors may refer to it as a $(k + 1)$-noncrossing diagram (see, e.g., [3]), all results in this paper can be easily adapted by shifting parameter k to $k + 1$. In Fig. 6 we present an example of a 2-noncrossing diagram and a binary 1-noncrossing diagram. Two arcs are *parallel* if they cover the same set of free sites. The concept of parallel arcs as defined here is a natural generalization of that concept as defined in [13, p. 35] since an arc (s_1, s_2) in a binary 1-noncrossing diagram is parallel to another arc (s'_1, s'_2) if and only if s_1 and s_2 are adjacent to s'_1 and s'_2, respectively.

Given an arc (s_1, s_2) in a diagram S, we can derive a new diagram S' with one less arc by applying one of the following two operations to (s_1, s_2). The first operation is called *deleting* the arc, and S' is obtained from S by simply removing the arc (s_1, s_2). In this case, the length of S' is the same as that of S while the number of free sites could be the same, or increase by one or two. The second operation is called *suppressing* the arc, and S' is obtained by removing (s_1, s_2) from S as well as removing any newly resulting free sites, and finally relabelling if necessary. Note that in this case the number of free sites in S' is the same as that of S while the length of S' could be the same, or decrease by one or two. See Fig. 6 for an example, where S' is obtained from S by suppressing the arc $(3, 8)$ and the length of S' decreases by one since site 3 is removed from S while site 8 is kept. For technical reasons, we use the convention that a sequence of operations could be an empty sequence.

The set $\mathcal{S}_n$ of non-trivial diagrams with length n has a natural poset structure under the relation $\subseteq$ which is defined as follows: $S \subseteq S'$ if S and S' have the same length, and each arc in S is also an arc in S'. Note that $S \subseteq S'$ holds if and only if S can be obtained from S' by a sequence of arc deletions. We let $\mathcal{S}_{n,k}$ denote the subposet of $\mathcal{S}_n$ under $\subseteq$ that consists of all possible k-noncrossing diagrams in $\mathcal{S}_n$. Note that $\mathcal{S}_{n,1}$ is precisely the poset of all secondary structures on linear molecules with length n as studied in [13, p. 33].

2.2. Simplicial complexes. We now review some facts concerning posets and simplicial complexes that we will require later. More details can be found in [2] and the references therein.

Let $P = (P, \leq)$ be a finite poset (partial ordered set). To ease the notation, for two elements x_1, x_2 in P with $x_1 \leq x_2$ and $x_1 \neq x_2$, we also write $x_1 < x_2$, or equivalently, $x_2 > x_1$. A totally ordered subset $x_0 < x_1 < \cdots < x_t$ is called a *chain* of *length* t. The *rank* of P is the maximum chain length taken over all chains in P. If all maximal chains have the same finite length then P is called *pure*. For $x \in P$, the *open interval* $P_{>x}$ in P is the set $\{y \in P : y > x\}$. Suppose $Q = (Q, \preceq)$ is another poset. Then the *direct product* $P \times Q$ of two posets is the Cartesian product set ordered by $(x, y) \leq (x', y')$ if $x \leq x'$ in P and $y \preceq y'$ in Q. A map $f : P \to Q$ is a *poset map* if it is *order-preserving*, that is, $x \leq y$ in P implies $f(x) \preceq f(y)$ in Q. A *poset isomorphism* is a bijective poset map.

A *simplicial complex* Δ on a finite vertex set V is a collection of nonempty subsets of V, where each subset is called a *face* of Δ, such that each nonempty subset of a face is also a face. The *face poset* $\mathbf{F}(\Delta) = (\Delta, \subseteq)$ of Δ is the set of faces in Δ ordered by inclusion. The *dimension* of a face is its cardinality (as a set) minus one, and the *dimension* of Δ is the size of a maximum face in Δ. Note that, in line with usual conventions, the dimension of an empty complex is -1. A face whose dimension is the same as that of Δ is known as a *facet* of Δ. Following [2], a d-dimensional simplicial complex is *pure* if every face is contained in a d-dimensional face. The complex consisting of all nonempty subsets of a $(d+1)$-element set is called the *d-simplex*. The geometric realization of a simplicial complex Δ is denoted by $|\Delta|$. A simplicial d-sphere is a simplicial complex whose geometric realization is homeomorphic to the d-dimensional sphere.

For two simplicial complexes Δ_1 and Δ_2 on two disjoint vertex sets, their *join* is the complex $\Delta_1 * \Delta_2 = \Delta_1 \cup \Delta_2 \cup \{F_1 \cup F_2 \,|\, F_1 \in \Delta_1 \text{ and } F_2 \in \Delta_2\}$. Given two nonempty spaces X and Y, their *join* $X * Y$ is the quotient space of $X \times Y \times I$ determined by the equivalence relation which identifies $(x, y_1, 0)$ with $(x, y_2, 0)$ and $(x_1, y, 1)$ with $(x_2, y, 1)$ for all x, x_1, x_2 in X and y, y_1, y_2 in Y. The following relation between the join operation on complexes and that of topological spaces is well known (see, e.g. Eq.(9.5) in [2]) :

$$|\Delta_1 * \Delta_2| \cong |\Delta_1| * |\Delta_2| \tag{2.1}$$

where $\cong$ denotes homeomorphism.

Given a poset P, its *order complex* $\Delta(P)$ is a simplicial complex whose vertices are the elements of P and whose faces are the finite nonempty chains of P. We shall use the following important link between direct products of posets and the join operation (see Theorem 5.1 in [22], also [16]): Given two posets $(P, \leq)$ and $(Q, \preceq)$ and $x \in P, y \in Q$, we have

$$|(P \times Q)_{>(x,y)}| \cong |P_{>x}| * |Q_{\succ y}|. \tag{2.2}$$

2.3. Adjacency matrices of diagrams. Let $m \geq 1$ be a positive integer. A *nonnegative integral symmetric* matrix $\mathbf{M} = (x_{i,j})$ of *order* m is a square matrix with m rows and m columns such that each entry $x_{i,j}$ is a nonnegative integer, and $x_{i,j} = x_{j,i}$ holds for all $1 \leq i, j \leq m$. If in addition each $x_{i,j}$ is either 0 or 1, then $\mathbf{M}$ is a symmetric $(0, 1)$-matrix. Note that all matrices considered in this paper are symmetric and nonnegative integral. A matrix is called *trivial* if all its elements are zero, and *non-trivial* otherwise.

For a square matrix $\mathbf{M} = (x_{i,j})$ of order m, the *diagonal elements* in $\mathbf{M}$ are the entries $x_{i,i}$ with $1 \leq i \leq m$, and the *semi-diagonal elements* are the superdiagonal entries $x_{i,i+1}$ with $1 \leq i < m$ and the subdiagonal entries $x_{i,i-1}$ with $1 < i \leq m$. Motivated by the terminology used in [7], the two elements $x_{1,m}$ and $x_{m,1}$ are referred to as the *rainbow elements*. Now, for four distinct integers a, b, c, d we say $\{a, b\}$ and $\{c, d\}$ are *crossing* if $\min\{a, b\} < \min\{c, d\} < \max\{a, b\} < \max\{c, d\}$ or $\min\{c, d\} < \min\{a, b\} < \max\{c, d\} < \max\{a, b\}$, two entries $x_{i,j}$ and $x_{p,q}$ in $\mathbf{M}$ are *crossing* if the index pairs $\{i, j\}$ and $\{p, q\}$ are crossing. If $\mathbf{M}$ does not contain $(k + 1)$ mutually crossing non-zero entries it will be referred to as a *k-noncrossing matrix*.

A matrix $A = (a_{i,j})$ is *dominated* by another matrix $B = (b_{i,j})$, written as $A \leq B$, if they have the same order m and $a_{i,j} \leq b_{i,j}$ holds for $1 \leq i, j \leq m$. For $m \geq 4$, let $\mathcal{M}_m$ be the non-empty set of symmetric non-trivial $(0, 1)$-matrices of order m in which all diagonal, semi-diagonal and rainbow elements are zero. Then $\mathcal{M}_m$ is a poset under the relationship $\leq$, where $A \leq B$ holds for matrices A and B in $\mathcal{M}_m$ if A is dominated by B. For $m \geq 4$ and $k \geq 1$, we let $\mathcal{M}_{m,k}$ be the subset of $\mathcal{M}_m$ consisting of all k-noncrossing matrices. Then $(\mathcal{M}_{m,k}, \leq)$ is a subposet of $(\mathcal{M}_m, \leq)$.

Now, given a diagram S with length n, we define its *adjacency matrix* $\mathbf{A}(S)$ to be the symmetric $(0, 1)$-matrix $(a_{i,j})$ of order n such that $a_{i,j}$ is 1 if either (i, j) or (j, i) is an arc. Note that both of the two rainbow elements of $\mathbf{A}(S)$ must be zero because the arc $(1, n)$ is not allowed in S by definition. For example, the adjacency matrix $\mathbf{A}(S') = (a_{i,j})$ of the 1-noncrossing diagram S' in $\mathcal{S}_{8,1}$ that is depicted in Fig. 6 is the symmetric $(0, 1)$-matrix of order 8 whose non-zero entries are $a_{1,7}, a_{7,1}, a_{2,4}$ and $a_{4,2}$. This implies that $\mathbf{A}(S')$ is a matrix in $\mathcal{M}_{8,1}$.

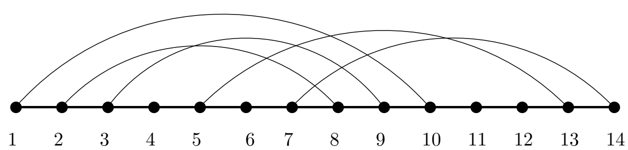
As the last example indicates, a number of properties of a given diagram are determined by its adjacency matrix. For instance, the number of arcs in S is half of the sum of the elements in $\mathbf{A}(S)$, and $S \subseteq S'$ if and only if $\mathbf{A}(S)$ is dominated by $\mathbf{A}(S')$. Moreover, the following result, whose proof is routine, shows that the map that associates a diagram with its adjacency matrix is in fact a poset isomorphism.

Proposition 2.1. *For $n \geq 4$, the map $S \to \mathbf{A}(S)$ is a poset isomorphism between $(\mathcal{S}_n, \subseteq)$ and $(\mathcal{M}_n, \leq)$. In addition, its restriction to $\mathcal{S}_{n,k}$ with $k \geq 1$ is a poset isomorphism between $(\mathcal{S}_{n,k}, \subseteq)$ and $(\mathcal{M}_{n,k}, \leq)$.* □

For later use, we let τ denote the map from $(\mathcal{S}_{n,k}, \subseteq)$ to $(\mathcal{M}_{n,k}, \leq)$ that associates a diagram with its adjacency matrix.

3. Block Matrices and Regular Diagrams. In this section we introduce and study a matrix which can be associated to a diagram, called its block matrix, which contains information concerning the structure of the diagram in a more condensed form than its adjacency matrix. Moreover, we show that for a special family of binary diagrams which we will call regular diagrams, they are k-noncrossing if and only if their block matrices are k-noncrossing.

Given a diagram S with length n, denote the number of free sites in S by $f = f_S \geq 0$. If $f > 0$, we let $u_1 < \cdots < u_f$ denote the set of free sites. Setting $u_0 = 0$ and $u_{f+1} = n+1$, then its *i-th block* $B_i = B_i(S)$ $(1 \leq i \leq f+1)$ consists of all (necessarily non-free) sites s in S with $u_{i-1} < s < u_i$. In other words, each maximal interval of non-free sites forms a block. For example, the interval consisting of the non-free sites 1, 2, and 3 is a block in the diagram in Fig. 7. Indeed, the diagram contains four free sites and hence it has five blocks. Note that a block can be the empty set, and that a diagram without any free sites has only one block. If an arc e is supported by a site in a block B, then we say that e and B are *incident*. The *block list* of S, denoted by $\mathcal{L}(S)$, is the list $(B_1, \ldots, B_{f+1})$ consisting of all blocks of S in the canonical order. The *block matrix* $\mathbf{B}(S)$ of S is the symmetric matrix with order $(f+1)$ in which the (i,j)-entry is the number of arcs incident with both B_i and B_j (see Fig. 7 for an example).



(i)

$$\begin{pmatrix} 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 3 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 \end{pmatrix}$$

(ii)

Fig. 7: Example of a diagram and its block matrix: (i) a 4-noncrossing diagram S; (ii) the block matrix $\mathbf{B}(S)$ associated with S. Since S contains four free sites: 4, 6, 11, and 12, it has five blocks: $B_1 = \{1,2,3\}$, $B_2 = \{5\}$, $B_3 = \{7,8,9,10\}$, $B_4 = \emptyset$, and $B_5 = \{13,14\}$.

The *number of crossings* in a diagram S is the total number of arc pairs in S that are crossing. Note that a diagram that is not k-noncrossing contains a set of $k+1$ arcs that are pairwise mutually crossing, and hence its number of crossings is at least $k(k+1)/2$. A crossing of two arcs e_1 and e_2 is called *local* if there exists a block B of S that contains two sites s_1 and s_2 such that e_1 and e_2 are supported by s_1 and s_2, respectively. A diagram is called *regular* if it is binary and does not contain any local crossings. For example, the diagram in Fig. 7 is not regular because $(2,8)$ and $(3,9)$ are two local crossing arcs. On the other hand, the diagram in Fig. 3(ii) is regular.

We now present two results relating properties of diagrams to those of their block matrices. The first one collects together some facts and its straightforward proof follows from the relevant definitions.

LEMMA 3.1. *For a diagram S, the following statements hold:*
(i) *S does not contain any degenerate arc if and only if all diagonal elements in $\mathbf{B}(S)$ are zero.*
(ii) *S does not contain any tiny arc if and only if all semi-diagonal elements in $\mathbf{B}(S)$ are zero.*
(iii) *S contains no parallel arcs if and only if $\mathbf{B}(S)$ is a $(0,1)$-matrix.*
(iii) *If S is binary, then S is proper if and only if all diagonal and rainbow elements in $\mathbf{B}(S)$ are zero.*
(v) *If S is proper and contains neither tiny nor parallel arcs, then $\mathbf{B}(S)$ is a non-trivial $(0,1)$-matrix in which all diagonal, semi-diagonal and rainbow elements are zero.* □

The second result shows that the block matrix of a binary k-noncrossing diagram is k-noncrossing.

LEMMA 3.2. *The block matrix of a binary k-noncrossing diagram is k-noncrossing.*

Proof. For simplicity, put $t = k + 1$. Suppose that S is a binary k-noncrossing diagram, and let f be the number of free sites in S. Then the block matrix $\mathbf{B}(S)$ of S can be written as $(b_{i,j})_{1\le i,j\le f+1}$. In addition, the list $\mathcal{L}(S)$ of the blocks contained in S can be written as $(B_1, \dots, B_{f+1})$.

We shall establish the lemma by contradiction. To this end, assume that $U = \{b_{r_1,c_1}, \dots, b_{r_t,c_t}\}$ is a set of mutually crossing non-zero entries contained in $\mathbf{B}(S)$. We claim that S contains a set of t pairwise crossing arcs, which contradicts the fact that S is k-noncrossing.

Since entries in U are mutually crossing, it follows that for $1 \le i < j \le t$, the integer pairs $\{r_i, c_i\}$ and $\{r_j, c_j\}$ are crossing. Therefore, $\{r_1, c_1, \dots, r_t, c_t\}$ is a set of $2t$ distinct integers. Since $\mathbf{B}(S)$ is symmetric, we may assume that $r_i < c_i$ holds for $1 \le i \le t$. In addition, relabelling the indices if necessary, we may assume that $r_1 < \cdots < r_t$.

Now for each $1 \le i \le t$, since $b_{r_i,c_i} > 0$, we fix an arc $e_i = (s_i, s'_i)$ such that s_i is contained in block B_{r_i} and s'_i is contained in block B_{c_i}. Then for $1 \le i < j \le t$, because b_{r_i,c_i} and b_{r_j,c_j} are crossing in the matrix $\mathbf{B}(S)$, we have $r_i < r_j < c_i < c_j$, and hence $s_i < s_j < s'_i < s'_j$. This implies e_i crosses e_j, and hence $\{e_i\}_{1\le i\le t}$ is a set of t mutually crossing arcs, as claimed. ∎

Note that the converse of Lemma 3.2 does not hold in general. For instance, the diagram S in Fig. 7 is 4-noncrossing while its block matrix $\mathbf{B}(S)$ is 2-noncrossing. However, the next result shows that the converse does hold for regular diagrams.

Proposition 3.3. *Suppose that S is a regular diagram. Then S is k-noncrossing if and only if $\mathbf{B}(S)$ is a k-noncrossing matrix.*

Proof. By Lemma 3.2 it follows that if S is k-noncrossing, then $\mathbf{B}(S)$ is k-noncrossing.

To see that the converse holds, for simplicity, put $t = k+1$ and let f be the number of free sites in S. Then the block matrix $\mathbf{B}(S)$ can be written as $(b_{i,j})_{1\le i,j\le f+1}$. In addition, the list $\mathcal{L}(S)$ of the blocks contained in S can be written as $(B_1, \dots, B_{f+1})$.

Now, suppose that S contains a set $\{(s_i, s'_i)\}_{1\le i\le t}$ of mutually crossing arcs. Then it suffices to establish the claim that $\mathbf{B}(S)$ must have t mutually crossing non-zero elements.

By swapping the indices if necessary, we may assume that $s_i < s_j$ holds for all $1 \le i < j \le t$. For each non-free site s in S, let $\alpha(s)$ be the index in $\{1, \dots, f + 1\}$ such that s is contained the block $B_{\alpha(s)}$ of S. Note that for two non-free sites $s < s'$, we have $\alpha(s) \le \alpha(s')$. In addition, if (s, s') is an arc in S, then $b_{\alpha(s),\alpha(s')} \ge 1$.

Now, consider the set $U = \{b_{\alpha(s_i),\alpha(s'_i)}\}_{1\le i\le t}$ of entries in $\mathbf{B}(S)$. Note first that each entry in U is non-zero. Moreover each pair of distinct elements in U are crossing. Indeed, fix two indices i and j with $1 \le i < j \le t$. Since (s_i, s'_i) and (s_j, s'_j) are crossing and $s_i < s_j$, we have $s_i < s_j < s'_i < s'_j$, and hence $\alpha(s_i) \le \alpha(s_j) \le \alpha(s'_i) \le \alpha(s'_j)$. Using the fact that S is regular, we can further conclude that

$$\alpha(s_i) < \alpha(s_j) < \alpha(s'_i) < \alpha(s'_j),$$

from which it follows that $\{\alpha(s_i), \alpha(s'_i)\}$ and $\{\alpha(s_j), \alpha(s'_j)\}$ are two pairs of crossing integers. Therefore U consists of t mutually crossing non-zero elements in $\mathbf{B}(S)$, which completes the proof of the claim. ∎

4. The Penner-Waterman Poset. In [13, p. 35] Penner and Waterman investigated the poset $\mathcal{B}^r_f$ of RNA secondary structures mentioned in the introduction.

In this section we introduce and study a generalisation of their poset for binary k-noncrossing diagrams.

To define this new poset we need some additional terminology. Given a non-negative integral matrix $\mathbf{M}$ of order m, we let

$$\mathbf{r}(\mathbf{M}) = \mathbf{p}(\mathbf{M}) + \mathbf{q}(\mathbf{M}), \tag{4.1}$$

be the *tautology number* of $\mathbf{M}$, where

$$\mathbf{p}(\mathbf{M}) = \sum_{1\le i<j\le m} \max\{0, x_{i,j} - 1\} \;\text{ and }\; \mathbf{q}(\mathbf{M}) = \sum_{1\le i<m} x_{i,i+1}. \tag{4.2}$$

In addition, given a diagram S, we define its *tautology number* to be $\mathbf{r}(\mathbf{B}(S))$. In particular, if S is 1-noncrossing, then $\mathbf{p}(\mathbf{B}(S))$ and $\mathbf{q}(\mathbf{B}(S))$ are the same as the values $p(S)$ and $q(S)$ as defined in [13, p.35], respectively, and $\mathbf{r}(\mathbf{B}(S))$ is the number of tautological arcs in S. Moreover, $\mathbf{r}(\mathbf{B}(S)) = 0$ holds if and only if S contains neither tiny nor parallel arcs. Finally, for $r \ge 0, m \ge 4$, and $k \ge 1$, we let $\mathcal{M}^r_{m,k}$ be the non-empty set of symmetric non-trivial non-negative integral k-noncrossing matrices of order m whose tautology number is less than or equal to r and in which all diagonal and rainbow elements are zero. Clearly, we have $\mathcal{M}^r_{m,k} \subseteq \mathcal{M}^{r+1}_{m,k}$ and $\mathcal{M}^r_{m,k} \subseteq \mathcal{M}^r_{m,k+1}$. In particular, all matrices in $\mathcal{M}^0_{m,k}$ are necessarily $(0,1)$-matrices and hence we have $\mathcal{M}^0_{m,k} = \mathcal{M}_{m,k}$.

Now, we let $\mathcal{P}^r_{f,k}$ be the set of all proper k-noncrossing diagrams S with f free sites and tautology number $\mathbf{r}(\mathbf{B}(S)) \le r$, and $\mathcal{B}^r_{f,k}$ be the subset consisting of all regular diagrams in $\mathcal{P}^r_{f,k}$. Note that for the special case $k = 1$, we have $\mathcal{P}^r_{f,1} = \mathcal{B}^r_{f,1}$, which is the set $\mathcal{B}^r_f$ introduced in [13, p.35]. More generally, we have $\mathcal{B}^r_{f,k} \subseteq \mathcal{P}^r_{f,k}$ in view of the following observation.

Lemma 4.1. *A regular diagram is proper.*

Proof. Suppose that S is a regular diagram. Denote the length of S by n and the number of free sites in S by f. Without loss of generality, we may assume that $n \ge 4$ and $f \ge 1$ as otherwise the lemma clearly holds.

First we shall show that S does not contain any degenerate arc. Suppose that this is not the case. Then there exists a block B of S such that the set $\Sigma(B)$ of arcs (s, s') in S with $\{s, s'\} \subseteq B$ is not empty. Now fix an arc $e_1 = (s_1, s'_1)$ in $\Sigma(B)$ so that the distance $|s_1 - s'_1|$ is minimum over all arcs in $\Sigma(B)$. We claim that s_1 and s'_1 are adjacent, that is, $s'_1 = s_1 + 1$, which leads to a contradiction because no arc in S is supported by two adjacent sites.

Suppose the claim is not true, and consider the site $s_2 := s_1 + 1$. Then s_2 is contained in B with $s_1 < s_2 < s'_1$. Let e_2 be the arc supported by s_2 and denote the other site supporting e_2 by s'_2. Since S is regular, e_1 and e_2 are not crossing, it follows that $s_1 \le s'_2 \le s'_1$ and hence $e_2 \in \Sigma(B)$. Moreover, this implies that $|s_2 - s'_2| < |s_1 - s'_1|$, a contradiction. Hence the claim holds, and therefore S does not contain any degenerate arc.

Let $\Sigma(S)$ be the set of the arcs in S that cover all free sites of S. It remains to prove that $\Sigma(S)$ is the empty set. Suppose this were not the case. Then fix an arc $e_3 = (s_3, s'_3)$ in $\Sigma(S)$ so that $s'_3 - s_3 \ge s' - s$ holds for each arc (s, s') in $\Sigma(S)$. Since $[s_3, s'_3]$ contains all free sites of S, it follows that s_3 is contained in $B_1(S)$, the first block of S, and that s'_3 is contained in $B_{f+1}(S)$, the last block of S. Moreover, neither 1 nor n is a free site, and thus site 1 is contained in $B_1(S)$ and site n is contained in $B_{f+1}(S)$.

Denote the site that is base-paired with 1 by s^*. Then s^* is not contained in $B_1(S)$ as S does not contain any degenerate arcs. In addition, we know that s^* is contained in $B_{f+1}(S)$ and $s^* \geq s'_3$ as otherwise $(1, s^*)$ and (s_3, s'_3) are two locally crossing arcs, a contradiction to the fact that S is regular. This implies that $s^* - 1 \geq s'_3 - s_3$, and hence $s^* - 1 = s'_3 - s_3$ in view of the maximality of (s_3, s'_3). It follows that $s_3 = 1$, and a similar argument shows that $s'_3 = n$. Thus $(1, n)$ is an arc in S, a contradiction to the fact that $1 < |s - s'| < n - 1$ holds for every arc (s, s') in a diagram of length n. Therefore, $\Sigma(S)$ is the empty set, which completes the proof. □

Next, we say $S \preceq S'$ holds for two diagrams S and S' in $\mathcal{P}^r_{f,k}$ if S can be obtained from S' by a sequence of arc suppressions. Note that the relation $\preceq$ is distinct from the poset relation $\subseteq$ as defined in Section 2.3. Moreover, it is straightforward to see that $S \preceq S'$ implies that $\mathbf{B}(S)$ is dominated by $\mathbf{B}(S')$. We now show that $(\mathcal{P}^r_{f,k}, \preceq)$ and $(\mathcal{B}^r_{f,k}, \preceq)$ are finite posets.

Proposition 4.2. *For $f \geq 2, r \geq 0, k \geq 1$ with $f + r \geq 3$, $(\mathcal{P}^r_{f,k}, \preceq)$ is a non-empty finite poset. Furthermore, $(\mathcal{B}^r_{f,k}, \preceq)$ is a subposet of $(\mathcal{P}^r_{f,k}, \preceq)$.*

Proof. When $r \geq 1$, it is straightforward to see that the set $\mathcal{B}^r_{f,k}$, and hence also the set $\mathcal{P}^r_{f,k}$, contains a diagram with one tiny arc for $f \geq 2$ and $k \geq 1$. On the other hand, when $f \geq 3$, both sets contain a diagram with one arc covering precisely two free sites for $r \geq 0$ and $k \geq 1$. Therefore, we know that both sets are non-empty for $f \geq 2, r \geq 0, k \geq 1$ with $f + r \geq 3$.

Since both sets are posets under the binary relation $\preceq$ and $\mathcal{B}^r_{f,k}$ is a subset of $\mathcal{P}^r_{f,k}$, it suffices to show that $\mathcal{P}^r_{f,k}$ is a finite set. This follows from the fact that the number of free sites f and the length n of a proper diagram S satisfy the following inequality:

$$n \leq \binom{f+3}{2} + 2\mathbf{p}(\mathbf{B}(S)). \tag{4.3}$$

To establish the inequality in Eq. (4.3), note first that after removing all but one arc from each parallel class of arcs, there exists at most one arc between each pair of blocks in S. Then the inequality follows because S contains precisely f free sites, the set of removed arcs contribute to at most $2\mathbf{p}(\mathbf{B}(S))$ non-free sites in S, and the remaining arcs contribute to at most $\binom{f+1}{2}$ non-free sites. □

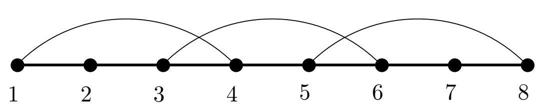


Fig. 8: A member of the infinite family of non-proper binary diagrams with two free sites defined in the text for $t = 4$.

For $f \geq 3, r \geq 0, k \geq 1$, we call poset $(\mathcal{B}^r_{f,k}, \preceq)$ the *Penner-Waterman* poset. Note that it is important to consider proper diagrams in the definition of the set $\mathcal{P}^r_{f,k}$. For example there exists infinitely many binary 3-noncrossing diagrams that have two free sites and $\mathbf{r}(\mathbf{B}(S)) = 0$. In particular, for each positive integer $t \geq 1$, let S_t be the diagram with length $4t$ that contains precisely all arcs of the form $(i, i+3)$ for every odd number i with $1 \leq i \leq 4t - 3$ (see Fig. 8 for the diagram with $t = 2$). Then S_t

contains precisely two free sites (the sites 2 and $4t-1$), and it is 3-noncrossing with $\mathbf{p}(\mathbf{B}(S_t)) = \mathbf{r}(\mathbf{B}(S_t)) = 0$.

5. An Equivalence Relation on Diagrams. In this section we present a characterization of the set of proper diagrams that have the same block matrix. In particular, we first define a certain equivalence relation $\sim$ on the set of proper diagrams, and then show that two proper diagrams have the same block matrix if and only if they are equivalent under $\sim$ (see Theorem 5.5).

We begin by defining $\sim$. Two proper diagrams S and S' are defined to be *equivalent*, denoted by $S \sim S'$, if they have the same length, and there exists a bijective map ϕ from the set of arcs in S to the set of arcs in S' that preserves free sites, that is, for each arc e in S, a free site s in S is covered by e if and only if s is covered by $\phi(e)$ in S'. See Fig. 9 for an example of two equivalent diagrams S_1' and S_2'. Note that in this example there are two such bijective maps from the arc set of S_1' to that of S_2': one maps arc $e_1 = (1, 8)$ in S_1' to arc $(1, 8)$ in S_2' and the other maps e_1 to arc $(2, 6)$. It is straightforward to check that $\sim$ is an equivalence relation on the set of proper diagrams, and that two equivalent diagrams have the same number of arcs.

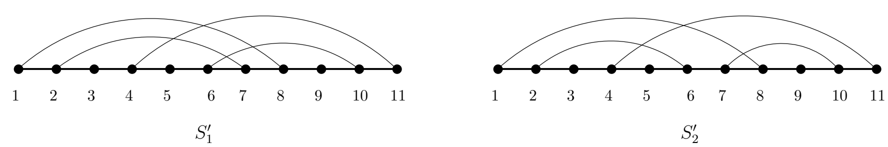


Fig. 9: Two equivalent proper diagrams S_1' and S_2' related by a single swap (S_2' can be obtained from S_1' by a swap $\epsilon[6]$ at site 6).

We now want to better understand when two proper diagrams are equivalent. To this end, we introduce a new operation on proper diagrams that preserves the $\sim$ relation. Suppose that s_1 and $s_2 = s_1 + 1$ are two adjacent non-free sites in a proper diagram S of length n, and denote the site base-paired with s_i by r_i for $i = 1, 2$. A *swap* $\epsilon = \epsilon[s_1]$ at s_1 generates a binary diagram $\epsilon(S)$ by replacing the two arcs supporting by s_1 and s_2 with two new arcs: one is supported by s_1 and r_2, and the other by s_2 and r_1 (see Fig. 9 for an example). Since S is proper, we have

$$1 < |s_1 - r_2| < n - 1 \quad \text{and} \quad 1 < |s_2 - r_1| < n - 1$$

and hence $\epsilon(S)$ is a binary digram. Note also that swapping is an involution, that is, swapping at s_1 twice results in the same diagram. We now show that $\epsilon(S)$ is a proper diagram that is equivalent to S, which has the same block matrix.

Lemma 5.1. *If ϵ is a swap on a proper diagram S, then $\epsilon(S)$ is a proper diagram. Moreover, $\epsilon(S) \sim S$, $\mathcal{L}(S) = \mathcal{L}(\epsilon(S))$, and $\mathbf{B}(S) = \mathbf{B}(\epsilon(S))$.*

Proof. Denote the site at which ϵ swaps by s_1. Put $s_2 = s_1 + 1$ and $S' = \epsilon(S)$. For $i = 1, 2$, let e_i be the arc in S supported by s_i and denote the other site supporting e_i by r_i. We shall assume that $e_1 = (r_1, s_1)$ and $e_2 = (s_2, r_2)$ since the other cases in which $e_1 = (s_1, r_1)$ or $e_2 = (r_2, s_2)$ (or both) can be established in a similar way.

Let $e_1' = (r_1, s_2)$ and $e_2' = (s_1, r_2)$. Then S' is obtained from S by replacing e_1 and e_2 by e_1' and e_2'. Note that the set of free sites covered by e_1 (i.e., those in $[r_1, s_1]$) is the same as the set covered by e_1' (i.e., those in $[r_1, s_2]$). Similarly, the set of sites covered by e_2 is the same as that covered by e_2'. Now let ϕ be the map that maps e_i

to e'_i for $i = 1, 2$ and maps each of the other arcs in S to the same arc in S'. Then ϕ is a bijection preserving free sites, and so $S \sim S'$.

Since S and S' have the same length and the same set of free sites, it follows that $\mathcal{L}(S) = \mathcal{L}(S')$. In addition, for two arbitrary blocks $B_i(S)$ and $B_j(S)$ in S, the number of arcs between them is the same as that in S', and so $\mathbf{B}(S) = \mathbf{B}(S')$. □

We now show that the swap operation can be used to convert a proper diagram into a canonical form.

LEMMA 5.2. *Suppose that (s_1, s_2) is an arc in a proper diagram S, and s'_i is a site in the block containing s_i for $i = 1, 2$. Then there exists a sequence of swaps $\epsilon_1, \dots, \epsilon_t$ for some $t \geq 0$ such that (s'_1, s'_2) is an arc in the proper diagram $\epsilon_t \epsilon_{t-1} \cdots \epsilon_1(S)$.*

Proof. Let B_i and B_j be the block containing s_1 and s_2, respectively. Note that the lemma clearly holds when $s'_1 = s_1$ and $s'_2 = s_2$ (by taking an empty sequence with $t = 0$). Hence in the remainder of the proof we assume that either $s'_1 \neq s_1$ or $s'_2 \neq s_2$.

Since S is proper and (s_1, s_2) is an arc, it follows $B_i \neq B_j$, and hence $|s^*_1 - s^*_2| > 1$ for each site s^*_1 in B_i and s^*_2 in B_j. As the case $s_2 \neq s'_2$ can be established in a similar manner, we assume $s_1 \neq s'_1$. In addition, we further assume $s_1 < s'_1$ as the proof of the other case $s_1 > s'_1$ is similar.

We now proceed by induction on $d = |s_1 - s'_1| + |s_2 - s'_2|$. For the base case $d = 1$ we have $s'_1 = s_1 + 1$, and hence the lemma follows by taking $t = 1$ and $\epsilon_1 = \epsilon[s_1]$.

Now suppose $d > 1$ and the lemma holds for two arbitrary sites $s^*_1 \in B_i$ and $s^*_2 \in B_j$ with $0 < |s_1 - s^*_1| + |s_2 - s^*_2| < d$. In particular, the lemma holds for $s''_1 = s'_1 - 1$ and $s''_2 = s'_2$. Therefore, there exists a sequence of swaps $\epsilon_1, \dots, \epsilon_t$ for some $t \geq 1$ such that (s''_1, s''_2) is an arc in the proper diagram $S'' = \epsilon_t \epsilon_{t-1} \cdots \epsilon_1(S)$. Since $|s''_1 - s'_1| + |s''_2 - s'_2| = 1$, by the base case there exists a swap ϵ such that (s'_1, s'_2) is an arc in the proper diagram $S' = \epsilon(S'')$. This completes the proof of the induction step, and hence the lemma. □

Using Lemma 5.2, we now show that two equivalent proper diagrams have the same block list, which is a key step for establishing the main result in this section. Note that the converse of this proposition clearly does not hold.

PROPOSITION 5.3. *If S and S' are two proper diagrams with $S \sim S'$, then $\mathcal{L}(S) = \mathcal{L}(S')$.*

Proof. Since $S \sim S'$, they have the same length, denoted by n, and also the same size, denoted by m. Thus it suffices to show that S and S' have the same set of free sites.

We proceed by induction on m. The base cases $m = 1$ follows by noting that both S and S' contain precisely the same set of non-free sites with cardinality two. Now assume $m > 1$ and that two equivalent proper diagrams with at most $m - 1$ arcs have the same set of free sites.

Since S contains two or more arcs, at least one block in the list $\mathcal{L}(S)$ is non-empty. Now let B_i be the first non-empty block in $\mathcal{L}(S)$, and denote the largest site in B_i by s_1. Let s_2 be the site so that (s_1, s_2) is an arc in S and denote the (necessarily non-empty) block containing s_2 by B_j. Since S is proper, it follows that $j > i$. Let s_3 be the smallest site in B_j.

Since S and S' are equivalent, there exists an arc (s'_1, s'_2) in S' such that the free sites in S contained in $[s_1, s_2]$ are the same as those in S' contained in $[s'_1, s'_2]$. Let B'_k and B'_l be the blocks in $\mathcal{L}(S')$ containing s'_1 and s'_2, respectively. Since $s_1 + 1$ is the smallest free site in $[s_1, s_2]$ and $[s'_1, s'_2]$ has the same set of free sites as that in $[s_1, s_2]$, it follows that the largest site in B'_k is s_1. Similarly, the smallest site in B'_l is s_3.

By Lemma 5.2, there exists a (possibly empty) sequence of swaps $\epsilon_1, \ldots, \epsilon_t$ for some $t \geq 0$ such that (s_1, s_3) is an arc in $S^* = \epsilon_t \cdots \epsilon_1(S)$. Similarly, there exists a (possibly empty) sequence of swaps $\epsilon'_1, \ldots, \epsilon'_{t'}$ for some $t' \geq 0$ such that (s_1, s_3) is an arc in $S'' = \epsilon_{t'} \cdots \epsilon_1(S')$. By Lemma 5.1 it follows that S^* and S'' are two equivalent proper diagrams. Consider the diagrams S^*_o and S''_o that are obtained from S^* and S'' respectively by suppressing the arc (s_1, s_3). Then S^*_o and S''_o are two equivalent proper diagrams with precisely $m-1$ arcs. Now the induction assumption implies that S^*_o and S''_o have the same set of free sites, from which it follows that S and S' have the same set of free sites. This completes the proof of the induction step and hence the proposition. □

The next result shows that the blocks of a binary diagram are determined by its block matrix (note that the converse clearly does not hold).

LEMMA 5.4. *Suppose that S and S' are two binary diagrams with $\mathbf{B}(S) = \mathbf{B}(S')$. Then S and S' have the same size and the same length. Furthermore, we have $\mathcal{L}(S) = \mathcal{L}(S')$.*

Proof. Let $(b_{i,j})_{1\leq i,j\leq (f+1)}$ be the elements in the block matrix $\mathbf{B} = \mathbf{B}(S) = \mathbf{B}(S')$, where $f+1$ is the order of $\mathbf{B}$. Then both S and S' contain f free sites. Next, the size of S is $\sum_{1\leq i\leq j\leq f+1} b_{i,j}$, the same as that of S'. Note that for a binary diagram, the number of its size is half of the difference between its length and the number of its free sites. Thus S and S' also have the same length. Finally, let $(B_1, \ldots, B_{f+1})$ and $(B'_1, \ldots, B'_{f+1})$ be the block lists of $\mathcal{L}(S)$ and $\mathcal{L}(S')$, respectively. Then for $1 \leq i \leq f+1$, we have

$$|B_i| = b_{i,i} + \sum_{1\leq j\leq f+1} b_{i,j} = |B'_i|,$$

from which $\mathcal{L}(S) = \mathcal{L}(S')$ follows. □

We now prove the main result of this section.

THEOREM 5.5. *Suppose that S and S' are two proper diagrams. Then*

$$\mathbf{B}(S) = \mathbf{B}(S') \quad \textit{if and only if} \quad S \sim S'.$$

Proof. Suppose that S and S' are two proper diagrams with $\mathbf{B}(S) = \mathbf{B}(S')$. Let $(b_{i,j})_{1\leq i,j\leq (f+1)}$ be the elements in the block matrix $\mathbf{B} = \mathbf{B}(S) = \mathbf{B}(S')$, where $f+1$ is the order of $\mathbf{B}$. Denote the set of indices (i,j) in $\mathbf{B}$ with $b_{i,j} > 0$ and $i \leq j$ by U.

By Lemma 5.4, S and S' have the same number of arcs, denoted by m, and the same length. Denoting the f free sites of S by $s_1 < \cdots < s_f$, then using Lemma 5.4 again we know that the free sites of S' are also $s_1, \ldots, s_f$.

Now, the set U induces a partition of the arcs in S as follows. For each (i,j) in U, let $A_{i,j}$ be the set of arcs in S between blocks $B_i(S)$ and $B_j(S)$. Then $A_{i,j}$ and $A_{i',j'}$ are disjoint for two distinct pairs (i,j) and (i',j') in U, and the set of arcs in S is the disjoint union $A_{i,j}$ over U in view of $\sum_{(i,j)\in U} b_{i,j} = m$. In other words, $\{A_{i,j}\}_{(i,j)\in U}$ is a partition of the set of arcs in S. Similarly, let $A'_{i,j}$ be the set of arcs in S' between blocks $B_i(S')$ and $B_j(S')$ so that $\{A'_{i,j}\}_{(i,j)\in U}$ is a partition of the set of arcs in S'.

For every (i,j) in U, and two arcs (r,s) in $A_{i,j}$ and (r',s') in $A'_{i,j}$, the set of free sites in $[r,s]$ is $\{s_{i+1}, s_{i+2}, \ldots, s_{j-1}\}$, which is also the set of free sites in $[r',s']$. Together with $|A_{i,j}| = a_{i,j} = |A'_{i,j}|$, this implies that we can fix a bijection $\phi_{i,j}$ from $A_{i,j}$ to $A'_{i,j}$ that preserves free sites. Now let ϕ be the map from the arcs in S to those in S' such that ϕ is $\phi_{i,j}$ when restricted to $A_{i,j}$ for each (i,j) in U. Then ϕ is a bijection between the arcs in S and those in S' that preserves free sites. Hence $S \sim S'$.

Conversely, suppose $S \sim S'$. Denote the number of free sites in S by f. Then we have $f \geq 1$ since S is proper. By Proposition 5.3, diagrams S and S' have the same block list, and hence also the same set of free sites, which we enumerate by $s_1 < s_2 < \cdots < s_f$. Thus $\mathbf{B}(S)$ and $\mathbf{B}(S')$ have the same order $f + 1$.

Let $(b_{i,j}) = \mathbf{B}(S)$ and $(b'_{i,j}) = \mathbf{B}(S')$. By Lemma 3.1 it follows that $b_{i,i} = b'_{i,i} = 0$ for $1 \leq i \leq f+1$. Now fix an arbitrary pair of indices $1 \leq i < j \leq f+1$. It suffices to show $b_{i,j} = b'_{i,j}$. To see this, note that $b_{i,j}$ is the number of arcs in S between block $B_i(S)$ and $B_j(S)$, which is precisely the number of arcs (s_1, s_2) in S such that the set of free sites in $[s_1, s_2]$ is $\{s_i, \ldots, s_{j-1}\}$. Since $S \sim S'$, there are precisely $b_{i,j}$ arcs (s'_1, s'_2) in S' such that the set of free sites in $[s'_1, s'_2]$ is $\{s_i, \ldots, s_{j-1}\}$. This implies $b_{i,j} = b'_{i,j}$, from which $\mathbf{B}(S) = \mathbf{B}(S')$ follows. ◻

6. Canonical Representatives. In this section, we show that there exists a unique regular diagram within each equivalence class of the equivalence relation $\sim$ on proper diagrams, and that this regular diagram has the minimum number of crossing arc pairs among all diagrams within that equivalence class (see Theorem 6.4).

To this end, first note that for a swap ϵ on a binary diagram S, S and $\epsilon(S)$ have the same number of non-local crossings. Moreover, the number of local crossings in $\epsilon(S)$ either increases or decreases by one. We therefore call a swap ϵ is called *strict* if $\epsilon(S)$ has one less crossing than S, or equivalently, $\epsilon(S)$ has one less local crossing than S. For example, the swap illustrated in Fig. 9 is strict.

Next, restricting the definition of regular, we call a block B in a binary diagram S regular if B does not contain two sites s_1 and s_2 for which there exists a pair of crossing arcs e_1 and e_2 in S that are supported by s_1 and s_2, respectively. In particular, a binary diagram S is regular if and only if every block in S is regular. The following result shows that blocks in proper diagrams that are not regular contain some special structures, which can be regarded as the 'obstruction' to their being regular.

Lemma 6.1. *A non-regular block in a proper diagram is incident with two adjacent arcs that are crossing.*

Proof. Suppose that B is a non-regular block in a binary diagram S and let b be the number of sites in B, so that $b \geq 2$. We establish the lemma by using induction on b.

The base case is $b = 2$, is straightforward to check. So assume that $b > 2$ and the lemma holds for all non-regular blocks containing at most $b - 1$ sites.

Denote the sites in B by $s_1 < \cdots < s_b$, enumerated from the smallest to the largest. Moreover, for $1 \leq i \leq b$, denote the site that is base-paired with s_i by s'_i, and let e_i be the arc supported by s_i and s'_i. Let Σ be the set of arcs which are supported by at least one site in B. Consider the arc e supported by s_b and put $\Sigma^* := \Sigma \setminus \{e\}$. Then we have the following two cases:

Case I: The arc set Σ^* does not contain a pair of crossing arcs.

By assumption, it follows that e_b crosses an arc e_i for some $1 \leq i \leq b - 1$. Now, assume $s_{b-1} < s'_{b-1}$. Then the interval $[s_{b-1}, s'_{b-1}]$ contains neither s_i nor s'_i for $1 \leq i < b - 1$. It follows that s'_b is not contained in $[s_{b-1}, s'_{b-1}]$ as otherwise e_b and e_i are not crossing for $1 \leq i \leq b - 1$, a contradiction. This implies that e_b is crossing with e_{b-1}.

So assume $s_{b-1} > s'_{b-1}$. Then the interval $[s'_{b-1}, s_{b-1}]$ contains both s_i and s'_i for $1 \leq i < b-1$. It follows that s'_b is contained in $[s'_{b-1}, s_{b-1}]$ as otherwise e_b and e_i are not crossing for $1 \leq i \leq b-1$, a contradiction. This again implies that e_b is crossing with e_{b-1}.

The induction step now follows immediately (note that the induction assumption is not required for establishing this case).

Case II: The arc set Σ^* contains a pair of crossing arcs.

Consider the proper diagram S' obtained from S by suppressing the arc e_b. Since S is proper, there is a block B' in S' that contains all the sites in B other than s_b. Denote the set of arcs which are supported by some site in B' by Σ'. Then B' is a non-regular block in S' with precisely $b-1$ sites. Thus by the induction assumption B' is incident with a pair of adjacent crossing arcs e and e' in S'. Since e and e' are obtained from two adjacent crossing arcs in S that are incident with B, the induction step follows. □

Remark: Using a more detailed analysis in Case II, the above argument can be extended to show that the last lemma also holds for binary diagrams.

The last result enables us to show that each proper diagram can be converted into a regular diagram within its equivalence class by applying a sequence of strict swaps.

PROPOSITION 6.2. *Given a proper diagram S, there exists a sequence of strict swaps $\epsilon_1, \ldots, \epsilon_t$ for some $t \geq 0$ such that $\epsilon_t \epsilon_{t-1} \cdots \epsilon_1(S)$ is a regular diagram that is equivalent to S.*

Proof. If S is regular, the proposition holds by taking $t = 0$. Hence we may assume in the remainder of the proof that S is not regular. Let b be the number of arc pairs in S that are locally crossing. Then we have $b \geq 1$ as S is not regular. We now establish the proposition by using induction on b.

For the base case $b = 1$, which implies that there exists a non-regular block B in S. By Lemma 6.1, there exist two adjacent sites s_1 and $s_2 = s_1 + 1$ in B so that the arc e_1 supported by s_1 is crossing with the arc e_2 supported by s_2. Since S is proper, by Lemma 5.1 we can apply a swap ϵ at s_1 to obtain a proper diagram $S' = \epsilon(S)$ with $S' \sim S$. Since e_1 and e_2 are crossing, it is straightforward to check that diagram S' contains one less local crossing than that of S, and hence S' is regular, completing the proof of the base case.

Now assume that $b > 1$ and the lemma holds for each proper diagram S which contains at most $b-1$ local crossing arc pairs. An argument similar to the base case shows that there exists a strict swap ϵ_1 so that $\epsilon_1(S)$ is a proper diagram which is equivalent to S and which has $b-1$ local crossing arc pairs. The proposition now follows by induction. □

To illustrate the last result, note that the proper diagram S_1 in Fig. 3 can be converted to the regular diagram S_2 in Fig. 3 by three strict swaps, consecutively acting on sites 1, 6 and 7 (see Fig. 9 where $\epsilon[1](S_1)$ and $\epsilon[6]\epsilon[1](S_1)$ are depicted as S'_1 and S'_2, respectively).

Now we show that regular diagrams are unique within any equivalence class of $\sim$.

LEMMA 6.3. *If S and S' are two regular diagrams with $S \sim S'$, then $S = S'$.*

Proof. Let S and S' be two regular diagrams with $S \sim S'$. Then they have the same length, denoted by n, and they contain the same number of arcs, denoted by m. Without loss of generality, we may assume that $n \geq 4$ as otherwise the lemma clearly holds.

By Proposition 5.3 we have $\mathcal{L}(S') = \mathcal{L}(S)$ (which we shall denote by $\mathcal{L}$), and it contains $f+1$ blocks for some $f \geq 1$ as S and S' are both proper in view of Lemma 4.1. Note that this implies that S and S' have the same set of free sites. Since $S \sim S'$, we can fix a bijection φ that maps each arc e in S to an arc $\varphi(e)$ such that a free site s in S is covered by e if and only if s is covered by $\varphi(e)$ in S'.

We now prove the lemma by induction on m. The base case is $m = 1$. Since S and S' have length n and have the same set of two non-free sites, it follows that $S = S'$ and hence the lemma follows. For induction step, assume $m > 1$ and the lemma holds for any two equivalent regular diagrams with at most $m - 1$ arcs.

Since $m > 1$, there exist at least two non-free sites in S. Denote the first non-free site in S by s_1, and let s_2 be the site in S so that (s_1, s_2) is an arc in S. Since S and S' have the same set of free sites, it follows that s_1 is also the first non-free site in S'. Let s'_2 be the site in S' so that (s_1, s'_2) is an arc in S'. Denote the block containing s_1 by B_i and the one containing s_2 by B_j. Then $1 \leq i < j \leq f + 1$ since S is proper and B_i is the first non-empty block in $\mathcal{L}$. Moreover, if (s''_1, s''_2) is the arc in S' that is the image of (s_1, s_2) under φ, then s''_1 is contained in B_i and s''_2 is contained in B_j because $[s_1, s_2]$ and $[s''_1, s''_2]$ contain the same set of free sites (see Fig. 10 for an illustration of the notation).

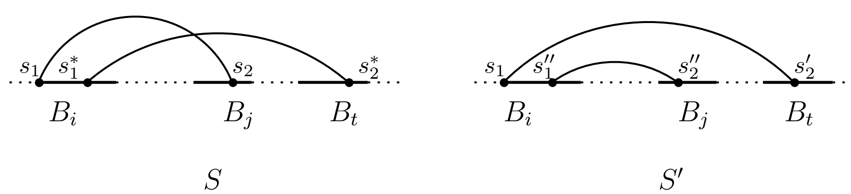


Fig. 10: An illustration for one step in the proof Lemma 6.3. Note that S and S' have the same set of blocks, among which only three are shown here.

Next we shall show that s'_2 is contained in B_j. Note that if $s_1 = s''_1$, then we have $s''_2 = s'_2$, and hence s'_2 is contained in B_j. Therefore we only need to consider the case $s_1 \neq s''_1$. This implies that $s_1 < s''_1 < s'_2$ holds because s_1 is the first non-free site and B_i is the first non-empty block which contains s_1 and s''_1 but not s_2. In addition, let B_t be the block in $\mathcal{L}$ that contains s'_2. Then we have $i < t \leq f + 1$ and so it remains to show $t = j$.

To this end, first note that if $t < j$, then $s_1 < s''_1 < s'_2 < s''_2$ and hence (s_1, s'_2) and (s''_1, s''_2) are two locally crossing arcs in S', a contradiction to the fact that S' is regular. On the other hand, if $j < t$, then consider the arc (s^*_1, s^*_2) in S such that (s^*_1, s^*_2) is mapped to (s_1, s'_2) by φ. Since $[s^*_1, s^*_2]$ and $[s_1, s'_2]$ contain the same set of free sites, it follows that s^*_1 is contained in block B_i and s^*_2 is contained in block B_t. Note that we may further assume that $s_1 < s^*_1$ because otherwise we have $s_1 = s^*_1$, and hence $s_2 = s^*_2$, from which $t = j$ follows. Together with $j < t$, this implies $s_1 < s^*_1 < s_2 < s^*_2$, and thus (s_1, s_2) and (s^*_1, s^*_2) are two locally crossing arcs in S, a contradiction to the fact that S is regular (see Fig. 10 for an illustration of this case). Therefore, we have $t = j$ and hence s'_2 is contained in B_j.

Our next step is to show that (s_1, s_2) is an arc contained in S'. To this end, it suffices to show $s_2' = s_2$. Denote the number of sites in B_j that are smaller than s_2 by b, and that are smaller than s_2' by b'. Moreover, let $r+1$ be the smallest site in B_j, that is, B_j contains $r+1$ but does not contain r. Note that for each site s_3 in block B_j with $s_3 > s_2$, there exists a site $s_3^* > s_3$ so that (s_3, s_3^*) is an arc in S since otherwise (s_1, s_2) and the arc supported by s_3 are local crossing, a contradiction. Therefore, the number of arcs (s, s^*) in S such that r is the largest free site in $[s, s^*]$ is $b+1$. A similar argument shows that the number of arcs (s', s'') in S' so that r is the largest free site in $[s', s'']$ is $b'+1$. Since S is equivalent to S', it follows that $b+1 = b'+1$ holds, and hence $s_2' = s_2$.

Noting that (s_1, s_2) is a common arc in S and S', we finally consider the two diagrams S_o and S_o' that are obtained from S and S' respectively by suppressing the arc (s_1, s_2). Then S_o and S_o' are two equivalent regular diagrams with $m-1$ arcs. By the induction assumption we have $S_o = S_o'$, and thus $S = S'$. This completes the proof of the induction step, from which the theorem follows. ∎

We now prove the main result of this section.

Theorem 6.4. *Given a proper diagram S, there exists a unique regular diagram S' with $S \sim S'$. Moreover, S is regular if and only if the number of crossings in S has the minimal number of crossings in its equivalence class.*

Proof. By Proposition 6.2, there exists a regular diagram S' that is equivalent to S. The uniqueness follows from Lemma 6.3.

It remains to show the second part of the theorem, that is, S is regular if and only if the number of crossings in S is less than or equal to that in each proper diagram S'' with $S'' \sim S$.

First, suppose that S is a regular diagram and assume that S' is a proper diagram S'' with $S'' \sim S$. By Proposition 6.2 and the first part of the theorem, diagram S can be obtained from S'' by a sequence of strict swaps, and hence the number of crossings contained in S is less than or equal to that contained in S''.

Conversely, suppose that the number of crossings in S is less than or equal to that in each proper diagram S'' with $S'' \sim S$. If S is not regular, then by the first part of the theorem there exists a regular diagram S^* that is equivalent to S. By Proposition 6.2 and the first part of the theorem, diagram S^* can be obtained from S by a sequence of strict swaps, and hence the number of crossings contained in S^* is less than that contained in S, a contradiction. Therefore S is regular. ∎

It is worth noting that combining Proposition 6.2 and Theorem 6.4 provides another characterisation of equivalence between proper diagrams, in addition to the one given in Theorem 5.5. The proof of this fact is straightforward and hence omitted here.

Corollary 6.5. *Suppose that S and S' are two proper diagrams. Then $S \sim S'$ if and only if there exists a sequence of swaps $\epsilon_1, \ldots, \epsilon_t$ for some $t \geq 0$ such that $S' = \epsilon_t \epsilon_{t-1} \cdots \epsilon_1(S)$* □

7. Poset Isomorphisms. In this section we study the two maps ρ and σ in Fig. 5 introduced in Section 1.2. In particular, we will prove the following result:

Theorem 7.1. *For $f \geq 3$, $r \geq 0$, and $k \geq 1$, the map*

$$\rho : (\mathcal{P}^r_{f,k}, \preceq) \to (\mathcal{M}^r_{f+1,k}, \leq) \; : \quad S \mapsto \mathbf{B}(S)$$

is a surjective poset homomorphism. Moreover, its restriction

$$\sigma : (\mathcal{B}^r_{f,k}, \preceq) \to (\mathcal{M}^r_{f+1,k}, \leq) \; : \quad S \mapsto \mathbf{B}(S)$$

is a poset isomorphism.

Using this theorem, we shall also show that in the case $r = 0$ the composition $\tau^{-1}\sigma$ in Fig. 5 gives a poset isomorphism between $(\mathcal{B}^0_{f,k}, \preceq)$ and $(\mathcal{S}_{f+1,k}, \subseteq)$ (see Theorem 7.4 below).

We begin by introducing two types of operations on diagrams which are motived by the construction in [13, Theorem 2]. Given a diagram S with length $n \geq 2$, the first operation creates its *dual* diagram S^* as follows. Denote the set of free sites in S by $F(S)$, and create a new set of sites $H(S)$ consisting of sites of the form $i + \frac{1}{2}$ for all $1 \leq i < n$. Then remove each site in $F(S)$, and label all newly created sites (i.e. those in $H(S)$) and relabel all other sites if necessary to obtain a diagram with length $2n - 1 - |F(S)|$ and $n - 1$ free sites. To illustrate this process, in Fig. 11 we depict the dual diagram S^* of the diagram S in Fig. 6.

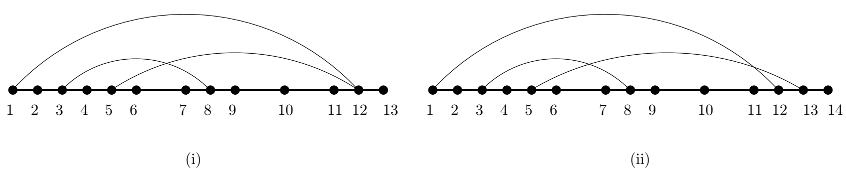


Fig. 11: Examples of dual and blow-up operations: (i) The dual of the diagram S in Fig. 6. (ii) The blow-up of the diagram in (i).

Since each arc (i, j) in S satisfies $1 < |i-j| < n-1$, the dual diagram S^* contains no tiny arcs since each arc in S^* covers at least two free sites. Moreover, no arc in S^* covers all of the free sites in S^*. In addition, note that both S and S^* have the same size, that is, the same number of arcs. The next technical lemma provides further connection between a diagram and its dual.

LEMMA 7.2. *Given a diagram S with length $n \geq 2$, we have $\mathbf{A}(S) = \mathbf{B}(S^*)$.*

Proof. Without loss of generality, suppose that the size of S is m for some $m \geq 1$ (as otherwise the lemma clearly follows). Let $(a_{i,j}) = \mathbf{A}(S)$ and $(b_{i,j}) = \mathbf{B}(S^*)$. By construction, diagram S^* has $f^* = n - 1 \geq 1$ free sites, and hence $(b_{i,j})$ has order n, the same as that of $(a_{i,j})$. Moreover, since the number of arcs in S is m and $\mathbf{B}(S^*)$ is symmetric, it follows that the sum of the elements $b_{i,j}$ in $\mathbf{B}(S^*)$ is $2m$, which is the same as the sum of the elements $a_{i,j}$ in $\mathbf{A}(S)$.

Because $\mathbf{A}(S)$ and $\mathbf{B}(S^*)$ are two symmetric non-negative integral matrices of order n whose sum of entries is the same, it suffices to show that for each $1 \leq i \leq j \leq n$, we have $b_{i,j} \geq a_{i,j}$. This is clearly the case if $a_{i,j} = 0$ and hence we may assume that $i < j$ and $a_{i,j} = 1$, that is, (i, j) is an arc in S. Now let (s, s') be the arc in S^* that is derived from (i, j) in S. Let u^*_t $(1 \leq t \leq f^*)$ be the t-th free site in S^* and put $u^*_0 = 0$. By construction, site s is between u^*_{i-1} and u^*_i, and hence is contained in block $B_i(S^*)$. Similarly, we know that site s' is contained in block $B_j(S^*)$. Thus (s, s') is an arc between $B_i(S^*)$ and $B_j(S^*)$, from which we have $b_{i,j} \geq 1$, as required. □

The second operation converts a non-binary diagram S into a binary one $\delta(S)$ as follows. Consider a site s in a diagram S supporting $b \geq 2$ arcs, that is, s is base-paired with b sites $s_1 < s_2 < \cdots < s_b$. The *blow up* at s results in the diagram $\delta_s(S)$ that is obtained from S by replacing the site s with b new sites $s'_1, s'_2, \ldots, s'_b$, and for $1 \leq i \leq b$, replacing the arc supported by s and s_i with a new arc supported by s'_i and

s_i. Finally all newly created sites are relabelled by consecutive integers and all other sites are relabelled if necessary. Note that each of the newly created sites supports precisely one arc, and hence the number of sites in $\delta_s(S)$ that support at least two arcs is one less than that in S. We now continue this process until a binary diagram, called the *blow up* of S and denoted by $\delta(S)$, is obtained. See Fig. 11 for an example. Note that $\mathbf{B}(S) = \mathbf{B}(\delta(S))$.

Using the dual and blow up operations, we now present a characterisation of matrices that can be realized as the block matrix of a proper diagram, which will be key in proving Theorem 7.1.

THEOREM 7.3. *Suppose that* $\mathbf{M}$ *is a symmetric non-negative non-trivial integral matrix. Then there exists a proper diagram* S *with* $\mathbf{B}(S) = \mathbf{M}$ *if and only if all diagonal and rainbow elements in* $\mathbf{M}$ *are zero. Moreover, if* $\mathbf{M}$ *is a* $(0,1)$*-matrix, then* S *contains no parallel arcs.*

Proof. The "only if" direction follows from Lemma 3.1. To establish the "if" direction, we shall first prove the following

Claim: Given a symmetric non-trivial $(0,1)$-matrix $(b_{i,j}) = \mathbf{B}$ of order $m \geq 1$ whose diagonal and rainbow elements are zero, there exists a proper diagram S containing no parallel arcs such that $\mathbf{B}(S) = \mathbf{B}$.

Proof of the Claim: Since $\mathbf{B}$ is non-trivial, it contains at least one non-zero element and hence by the assumptions of the claim we have $m \geq 3$.

Let $H = \{1 \leq i < m : b_{i,i+1} \geq 1\}$ be the index set of the non-zero superdiagonal elements in $\mathbf{B}$. Consider the matrix $\mathbf{B}'$ obtained from $\mathbf{B}$ by replacing both $b_{i,i+1}$ and $b_{i+1,i}$ with zero for each index i in H. Then all diagonal, semi-diagonal and rainbow elements in $\mathbf{B}'$ are zero. By Proposition 2.1, there exists a diagram S' with $\mathbf{A}(S') = \mathbf{B}'$. Now let S^* be the dual of S', and let δ be the blow up of S^* so that $S'' = \delta(S^*)$ is a binary diagram. Then we have

$$\mathbf{B}(S'') = \mathbf{B}\left(\delta(S^*)\right) = \mathbf{B}(S^*) = \mathbf{A}(S') = \mathbf{B}',$$

where the third equality follows from Lemma 7.2. Using Lemma 3.1 it follows that S'' is a proper diagram containing neither tiny nor parallel arcs.

Now for each index i in H, insert a new site a_i in block $B_i(S'')$ and a new site a_j in block $B_{i+1}(S'')$, and add an arc between these two newly added sites. Finally, relabel all the sites to obtain a diagram.

Let S be the diagram resulting from S'' after performing the above operation for each of the indices in H. Then, by construction, S is a proper diagram which has the same number of free sites as that of S'', such that S does not contain any parallel arcs. Moreover, we have $\mathbf{B}(S) = \mathbf{B}$, from which the claim follows. □

Now we proceed to establish the "if" direction. To this end, assume that $(x_{i,j}) = \mathbf{M}$ is a symmetric non-negative non-trivial integral matrix of order m whose diagonal and rainbow elements are zero. Let $\mathbf{M}' = (x'_{i,j})$ be the maximal symmetric $(0,1)$-matrix of order m dominated by $\mathbf{M}$, that is, where $x'_{i,j} = 1$ if and only if $x_{i,j} \geq 1$ holds. Then the diagonal and rainbow elements in $\mathbf{M}'$ are 0. By the **Claim**, there exists a diagram S' with $\mathbf{B}(S') = \mathbf{M}'$. Let

$$A = \{(i,j) \,:\, 1 \leq i < j \leq m \;\text{ and }\; x_{i,j} - x'_{i,j} \geq 1\}$$

be the set of positions above the diagonal in which the element in $\mathbf{M}$ differs from that in $\mathbf{M}'$.

For each position (i, j) in A, put $t = x_{i,j} - x'_{i,j}$. Then we have $t \geq 1$. Now insert t new sites $a_1, \ldots, a_t$ in block B_i and t new sites $b_1, \ldots, b_t$ in block B_j, relabel all of the sites, and for $1 \leq p \leq t$, add an arc between the two newly added sites a_p and b_p. Denote the resulting binary diagram obtained from S' after completing the above operation for each position in A by S. Then by construction it follows that S is binary diagram with $\mathbf{B}(S) = \mathbf{M}$. By Lemma 3.1 we can further conclude that S is a proper diagram, from which the theorem follows. □

Using this last result, we now prove Theorem 7.1.

Proof of Theorem 7.1: Given a diagram S in $\mathcal{P}^r_{f,k}$, we first show that $\mathbf{B}(S)$ is contained in $\mathcal{M}^r_{f+1,k}$. Indeed, because S contains f free sites, the order of $\mathbf{B}(S)$ is $f+1$. As S is a proper diagram with at least one arc, $\mathbf{B}(S)$ is a non-trivial symmetric non-negative integer matrix, and by Lemma 3.1 all diagonal and rainbow elements in $\mathbf{B}(S)$ are zero. Since S is k-noncrossing, by Lemma 3.2 it follows that $\mathbf{B}(S)$ is also k-noncrossing. Moreover, by $\mathbf{r}(\mathbf{B}(S)) = \mathbf{r}(S) \leq r$ we have $\mathbf{B}(S) \in \mathcal{M}^r_{f+1,k}$, as claimed. Therefore, ρ is indeed a poset homomorphism from $(\mathcal{P}^r_{f,k}, \preceq)$ to $(\mathcal{M}^r_{f+1,k}, \leq)$.

The next step is to show that the map ρ is surjective. To this end, fix a matrix $\mathbf{M}$ in $\mathcal{M}^r_{f+1,k}$. Since $\mathbf{M}$ is a symmetric non-negative integer matrix whose diagonal and rainbow entries are zero, by Theorem 7.3 there exists a proper diagram S with $\mathbf{B}(S) = \mathbf{M}$. Note that S contains precisely f free sites. By Theorem 6.4, we may assume that S is regular as otherwise we can replace it with the regular diagram in its equivalence class. Since $\mathbf{B}(S)$ is k-noncrossing and S is regular, by Proposition 3.3 it follows that S is also k-noncrossing. Together with $\mathbf{r}(S) = \mathbf{r}(\mathbf{B}(S)) \leq r$, we conclude that S is contained in $\mathcal{P}^r_{f,k}$, and hence the map ρ is surjective, as required.

The last step is to show that map σ is a poset isomorphism. Since ρ is surjective, by Theorems 5.5 and 6.4 it follows that map σ is a surjective poset homomorphism between $(\mathcal{B}^r_{f,k}, \preceq)$ and $(\mathcal{M}^r_{f+1,k}, \leq)$. Moreover, this map is injective by Theorems 5.5 and 6.4. □

Rephrased in our terminology, Penner and Waterman established a canonical isomorphism between the poset $(\mathcal{B}^0_{f,1}, \preceq)$, which consists of binary 1-noncrossing diagrams with f free sites and containing neither parallel nor tiny arcs, and the poset $(\mathcal{S}_{f+1,1}, \leq)$, which consists of all 1-noncrossing diagrams with at least one arc and length $f+1$ [13, Theorem 2]. We now conclude this section by using Theorem 7.1 to generalize this result to noncrossing diagrams (cf. Fig. 5).

Theorem 7.4. *For $f \geq 3$ and $k \geq 1$, the map*

$$\tau^{-1}\rho : (\mathcal{P}^0_{f,k}, \preceq) \to (\mathcal{S}_{f+1,k}, \subseteq) \;:\; S \mapsto \mathbf{A}^{-1}(\mathbf{B}(S))$$

is a surjective poset homomorphism. Moreover, its restriction to regular diagrams

$$\tau^{-1}\sigma : (\mathcal{B}^0_{f,k}, \preceq) \to (\mathcal{S}_{f+1,k}, \subseteq) \;:\; S \mapsto \mathbf{A}^{-1}(\mathbf{B}(S))$$

is a poset isomorphism.

Proof. This clearly follows from Proposition 2.1, Theorem 7.1, and the fact that $\mathcal{M}_{f+1,k} = \mathcal{M}^0_{f+1,k}$. □

Note that since $\mathcal{P}^0_{f,1} = \mathcal{B}^0_{f,1}$, the fact that $\mathcal{P}^0_{f,1}$ and $\mathcal{S}_{f+1,1}$ are isomorphic [13, Theorem 2] is also a consequence of the last result.

8. Spaces of k-noncrossing Diagrams. In this section we prove our main results. We first investigate some properties of the poset $(\mathcal{S}_{m,k}, \subseteq)$, $m \geq 2k+1$, as defined in Section 2.1. To do this we shall use a generalisation of triangulations mentioned in the introduction called k-triangulations (also known as multitriangulations) [5, 11, 21], whose definition we now recall.

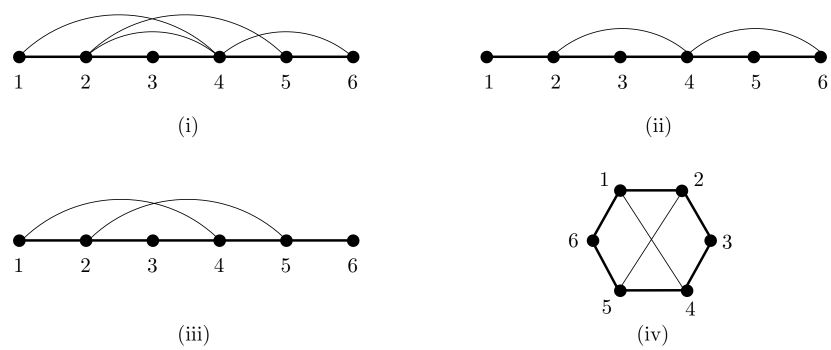


Fig. 12: Examples of diagrams and k-triangulations: (i)A diagram S in $\mathcal{S}_{6,2}$; (ii) A diagram S_1 in $\mathcal{S}^*_{6,2}$; (iii) A diagram S_2 in $\mathcal{S}^o_{6,2}$. Note that both S_1 and S_2 are also diagrams in $\mathcal{S}_{6,2}$. Moreover, $\kappa(S) = (S_1, S_2)$ holds for the map κ defined in the proof of Lemma 8.1. (iv) A face T in $\mathcal{T}_{6,2}$. It consists of diagonals $1-4$ and $2-5$, both of which are 2-relevant. Note that $\theta(T) = S_2$ holds for the map θ in Lemma 8.2.

Consider the convex m-gon with vertices $\{1, 2, \ldots, m\}$. A diagonal between two vertices i and j in the m-gon, denoted by $i - j$, is called *k-relevant* if the length of the shortest path between these two vertices in the m-gon is greater than k, that is, $k < |i-j| < m-k$ holds (see Fig. 12(iv) for an example). Clearly, each diagonal in a set of $(k+1)$ pairwise crossing diagonals must be k-relevant. Denote the set of k-relevant diagonals in the m-gon by $\Gamma_{m,k}$, so that each set of $(k+1)$ pairwise crossing diagonals is a subset of $\Gamma_{m,k}$, and let $\mathcal{T}_{m,k}$ be the simplicial complex with vertex set $\Gamma_{m,k}$ whose faces are the nonempty subsets of $\Gamma_{m,k}$ which do not contain $(k+1)$ pairwise crossing diagonals. A maximal face in $\mathcal{T}_{m,k}$ is called a *k-triangulation of the m-gon* [21] . For example, the face depicted in Fig. 12(iv) is a 2-triangulation of the 6-gon. Note that some authors use the term k-triangulation in a slightly different way, allowing diagonals that are not necessarily k-relevant (see, e.g. [15]).

Motivated by these definitions, we say an arc $e = (s, s')$ in a diagram with length m is k-relevant if $k < |s - s'| < m - k$. Let $\mathcal{S}^o_{m,k}$ be the set containing all diagrams S in $\mathcal{S}_{m,k}$ such that every diagonal in S is k-relevant, and $\mathcal{S}^*_{m,k}$ denote the set consisting of all diagrams S in $\mathcal{S}_{m,k}$ in which no diagonal in S is k-relevant. See Fig 12(ii-iii) for examples of diagrams in $\mathcal{S}^*_{6,2}$ and $\mathcal{S}^o_{6,2}$. Note that $\mathcal{S}^*_{m,1} = \emptyset$ and $\mathcal{S}^o_{m,1} = \mathcal{S}_{m,1}$. Moreover, $\mathcal{S}^*_{m,k}$ and $\mathcal{S}^o_{m,k}$ are two disjoint subposets of $\mathcal{S}_{m,k}$ under $\subseteq$.

The arc set of any diagram S in $\mathcal{S}_{m,k}$ can be partitioned into two subsets: the one that contains all k-relevant arcs in S and the other its complement. In order to deal with the case that one of these two subsets is empty, we extend the posets $\mathcal{S}^*_{m,k}$ and $\mathcal{S}^o_{m,k}$ by adding a new bottom element to each of them, which we denote by 0^* and 0^o, respectively. We denote these new posets by $\hat{\mathcal{S}}^*_{m,k}$ and $\hat{\mathcal{S}}^o_{m,k}$, respectively. Note that we are assuming that 0^o is distinct from 0^*, and hence $\hat{\mathcal{S}}^*_{m,k}$ and $\hat{\mathcal{S}}^o_{m,k}$ are disjoint.

The next lemma will allow us to reduce the problem of understanding the topology of $|\Delta(\mathcal{S}_{m,k})|$ to that of understanding the topology of $|\Delta(\mathcal{S}^*_{m,k})|$ and $|\Delta(\mathcal{S}^o_{m,k})|$.

Lemma 8.1. *For $k \geq 1$ and $m \geq 2k+1$, the poset $\mathcal{S}_{m,k}$ is isomorphic to the open interval $(\hat{\mathcal{S}}^*_{m,k} \times \hat{\mathcal{S}}^o_{m,k})_{>(0^*,0^o)}$. Moreover, we have*

$$|\Delta(\mathcal{S}_{m,k})| \cong |\Delta(\mathcal{S}^*_{m,k})| * |\Delta(\mathcal{S}^o_{m,k})|. \tag{8.1}$$

Proof. First, consider the map κ_* that takes a diagram S in $\mathcal{S}_{m,k}$ to the diagram $\kappa_*(S)$ in $\hat{\mathcal{S}}^*_{m,k}$ that consists of all arcs e in S such that e is not k-relevant. In case each of the arcs in S is k-relevant, we set $\kappa_*(S) = 0^*$. Similarly, let κ_o be the map that takes a diagram S in $\mathcal{S}_{m,k}$ to the diagram $\kappa_o(S)$ in $\hat{\mathcal{S}}^o_{m,k}$ that consists of all k-relevant arcs in S or to 0^o if none of the arcs in S is k-relevant. Then it is straightforward to check that κ_* and κ_o are both poset homomorphisms.

Now consider the map κ that takes a diagram S in $\mathcal{S}_{m,k}$ to $(\kappa_*(S), \kappa_o(S))$. See Fig. 12(i-iii) for an example in which $\kappa(S) = (S_1, S_2)$. Then κ is a poset homomorphism from $\mathcal{S}_{m,k}$ to $\hat{\mathcal{S}}^*_{m,k} \times \hat{\mathcal{S}}^o_{m,k}$. Moreover, since S contains at least one arc, it follows that $(\kappa_*(S), \kappa_o(S)) \neq (0^*, 0^o)$.

On the other hand, given a pair $(S_1, S_2) \in \hat{\mathcal{S}}^*_{m,k} \times \hat{\mathcal{S}}^o_{m,k}$ that is distinct from $(0^*, 0^o)$, we consider the necessarily non-trivial diagram S that is obtained by taking the union of the arcs in S_1 and S_2. Then S is a diagram in $\mathcal{S}_{m,k}$ since S_1 contains no k-relevant arc, and hence no arc in S_1 can be contained in a set of $(k+1)$ pairwise crossing arcs. Furthermore, by construction we have $\kappa(S) = (S_1, S_2)$. Therefore κ is a surjective poset homomorphism from $\mathcal{S}_{m,k}$ to $(\hat{\mathcal{S}}^*_{m,k} \times \hat{\mathcal{S}}^o_{m,k})_{>(0^*,0^o)}$. Note that given two distinct diagrams S and S' in $\mathcal{S}_{m,k}$, there exists at least one arc that is contained in one but not both diagrams, and hence $\kappa(S) \neq \kappa(S')$ follows. This implies that κ is also injective, and thus κ is an isomorphism.

Finally, we have

$$\begin{aligned} |\Delta(\mathcal{S}_{m,k})| &\cong |\Delta\big((\hat{\mathcal{S}}^*_{m,k} \times \hat{\mathcal{S}}^o_{m,k})_{>(0^*,0^o)}\big)| \cong |\Delta\big((\hat{\mathcal{S}}^*_{m,k})_{\supset 0^*}\big)| * |\Delta\big((\hat{\mathcal{S}}^o_{m,k})_{\supset 0^o}\big)| \\ &\cong |\Delta(\mathcal{S}^*_{m,k})| * |\Delta(\mathcal{S}^o_{m,k})|. \end{aligned}$$

Here the second $\cong$ follows from Eq. (2.2), and the third $\cong$ follows from the fact that $(\hat{\mathcal{S}}^*_{m,k})_{\supset 0^*}$ and $(\hat{\mathcal{S}}^o_{m,k})_{\supset 0^o}$ are isomorphic to $\mathcal{S}^*_{m,k}$ and $\mathcal{S}^o_{m,k}$, respectively. □

In view of the last lemma, the topology of $|\Delta(\mathcal{S}_{m,k})|$ is determined by the topology of $|\Delta(\mathcal{S}^*_{m,k})|$ and $|\Delta(\mathcal{S}^o_{m,k})|$. It is straightforward to see that $|\Delta(\mathcal{S}^*_{m,k})|$ is a simplex of dimension $m(k-1)-1$. To obtain the topology of $|\Delta(\mathcal{S}^o_{m,k})|$, we define a natural map θ which takes any face T in the face poset $\mathbf{F}(\mathcal{T}_{m,k})$ of $\mathcal{T}_{m,k}$ with diagonal set $\{i_1 - j_1, \cdots, i_t - j_t\}$ to the diagram $\theta(T)$ in $\mathcal{S}^o_{m,k}$ with arc set $\{(i_1, j_1), \cdots, (i_t, j_t)\}$. For example, θ maps the face in Fig. 4(v) to the diagram in Fig. 4(iii). We now show that this yields a poset isomorphism.

Lemma 8.2. *For two integers $k \geq 1$ and $m \geq 4$ with $m \geq 2k+1$, the map θ induces a poset isomorphism from the face poset $\mathbf{F}(\mathcal{T}_{m,k})$ to $\mathcal{S}^o_{m,k}$. Moreover, the simplicial complex $\Delta(\mathcal{S}^o_{m,k})$ is a simplicial sphere of dimension $k(m-2k-1)-1$.*

Proof. It is straightforward to verify that θ is indeed a poset isomorphism. Therefore $\Delta(\mathcal{S}^o_{m,k})$ is isomorphic to $\Delta(\mathbf{F}(\mathcal{T}_{m,k}))$. Note that $\Delta(\mathbf{F}(\mathcal{T}_{m,k}))$ is the (first) barycentric subdivision of $\mathcal{T}_{m,k}$ and hence it is isomorphic to $\mathcal{T}_{m,k}$ (see, e.g. [2, p. 1844]). The lemma now follows from the fact that $\mathcal{T}_{m,k}$ is a simplicial sphere with dimension $k(m-2k-1)-1$ (see, e.g. Statement 1.3 and Theorem 1.1 in [21]). □

Since $\mathcal{S}_{m,1} = \mathcal{S}^o_{m,1}$ and $\mathcal{T}_{m,1}$ is the arc poset $\mathcal{T}_m$ of triangulations of an m-gon mentioned in Section 1, note that Lemmas 8.1 and 8.2 can be regarded as a generalization of the result relating 1-noncrossing diagrams to triangulations of a polygon as stated in [13, Theorem 2 and Proposition 3].

We now determine the topology of $|\Delta(\mathcal{S}_{m,k})|$. Note that the fact that $|\Delta(\mathcal{S}_{m,1})|$ is a topological sphere of dimension $m-4$ as established in [13] is a special case of the following result with $k=1$.

PROPOSITION 8.3. *For any two integers $k \geq 1$ and $m \geq 4$ with $m \geq 2k+1$, the poset $\mathcal{S}_{m,k}$ is pure and of rank $2k(m-k)-k-m$. Moreover, $|\Delta(\mathcal{S}_{m,k})|$ is homeomorphic to the join of a simplicial sphere of dimension $k(m-2k-1)-1$ and an $(m(k-1)-1)$-simplex.*

Proof. Since $\mathcal{S}^o_{m,k}$ and $\mathcal{S}^*_{m,k}$ are both pure, by Lemma 8.1 it follows that the poset $\mathcal{S}_{m,k}$ is pure and of rank $2k(m-k)-k-m$. The proposition now follows from Lemmas 8.1 and 8.2, and the fact that $\Delta(\mathcal{S}^*_{m,k})$ is an $(m(k-1)-1)$-simplex. □

Using Theorem 7.4 and Proposition 8.3, we immediately obtain our two main results as stated in Section 1, the first of which follows immediately:

THEOREM 1.1. *For two integers $k \geq 1$ and $f \geq 3$ with $f \geq 2k$, $|\Delta(\mathcal{B}^0_{f,k})|$ is the join of a simplicial sphere of dimension $k(f-2k)-1$ and an $((f+1)(k-1)-1)$-simplex.* □

THEOREM 1.2. *For any $r \geq 0$, $f \geq 3$ and $k \geq 1$ with $f \geq 2k$, the poset $(\mathcal{B}^r_{f,k}, \preceq)$ is pure and of rank $k(2f-2k+1)+r-f-1$.*

Proof. By Proposition 8.3 and Theorem 7.4, we know that $(\mathcal{B}^0_{f,k}, \preceq)$ is pure and of rank $2k(f-k)+k-f-1$. Now suppose that $S_1 \prec \cdots \prec S_t$ is a maximal chain in $\mathcal{B}^r_{f,k}$ for some $t>0$. Then we have $\mathbf{r}(S_t)=r$ since otherwise there exists a diagram S^*_t in $\mathcal{B}^r_{f,k}$ with $S_t \prec S^*_t$, a contradiction. Next, for each $1<i\leq t$, diagram S_i contains precisely one more arc than S_{i-1}. Thus we have $t>r$. In addition, this maximal chain induces precisely one maximal chain $S'_1 \prec \cdots \prec S'_{t-r}$ in $(\mathcal{B}^0_{f,k}, \preceq)$ by removing all tiny arcs, and all but one arc in each set of parallel arcs. Therefore, the length of each maximal chain in $\mathcal{B}^r_{f,k}$ is precisely r plus the length of a maximal chain in $\mathcal{B}^0_{f,k}$, from which the theorem immediately follows. □

9. Discussion. Using the topology of $|\Delta(\mathcal{B}^0_{f,1})|$ and the fact that the natural inclusion $\mathcal{B}^r_{f,1} \subseteq \mathcal{B}^{r+1}_{f,1}$ is a chain homotopy, in [13, Theorem 7] Penner and Waterman show that $|\Delta(\mathcal{B}^r_{f,1})|$ has the homology of a $(f-3)$-dimensional sphere for $f\geq 3$ and $r \geq 0$. It would therefore be of interest to see whether or not the following holds: For any $r\geq 0$, $f \geq 3$ and $k\geq 1$, $|\Delta(\mathcal{B}^r_{f,k})|$ has the same homology as the join of a simplicial sphere of dimension $k(f-2k)-1$ and an $((f+1)(k-1)-1)$-simplex. One approach to try proving this would be to first understand whether or not the natural inclusion $\mathcal{B}^r_{f,k} \subseteq \mathcal{B}^{r+1}_{f,k}$ is a chain homotopy.

Our results also lead to several interesting counting problems. For example, can formulae be found for the number of elements in $\mathcal{B}^r_{f,k}$ or $\mathcal{P}^r_{f,k}$? In addition, using Lemma 8.2 and [21, Theorem 1.2] (see,also [9, 10]) we can give a formula for the number of facets in $\Delta(\mathcal{S}^o_{m,k})$. It would be interesting to see whether Theorem 7.4 and Lemma 8.1, could be used together with this formula to determine the number of facets in $\Delta(\mathcal{B}^0_{f,k})$.

Finally, it could be of interest to investigate how the spaces studied here might help to understand properties of structures of RNA molecules in more practical applications. For example, although it is known that finding minimal energy pseudoknots is NP-complete under typical RNA minimum free energy models (see e.g. [1]), there are efficient algorithms for restricted classes of pseudoknots (see e.g. [18]). Hence it could be worth investigating if there is any relationship between the Penner-Waterman poset and collections of RNA structures satisfying such restrictions, e.g. genus restricted structures [18] or grammar-based structures (see e.g. [4, 12]). Note that multitriangulations have connections with several combinatorial structures such as polyonimoes and twisted surfaces [15], which indicates that there may be some interesting relationships to uncover.

In another direction it could be interesting to see if our results might be used to help define and study combinatorial landscapes of k-noncrossing RNA structures. Combinatorial landscape theory involves the study of configuration spaces (e.g. the space of RNA sequences with fixed length), that come equipped with some notion of adjacency (e.g. RNA sequences differing in one nucleotide are adjacent), on which some fitness map is defined that assigns a real number to each element in the space (e.g. the energy of a minimum free energy structure for an RNA sequence) [19]. This concept is useful in, for example, combinatorial optimization where it can be used to design algorithms for finding (locally) optimal elements in the underlying space. There is a natural notion of adjacency for multitriangulations that is given in terms of "flipping" around an edge in a multitriangulation to give another multitriangulation (this generalizes the well-known notion of flippings in triangulations – see e.g. [20]). Moreover, any two multitriangulations in $\mathcal{T}_{m,k}$ can be converted from one to the other through a sequence of flips (see e.g. [15] and the references therein). Thus, it would be interesting to explore if these results coupled with our above observations concerning multitriangulations might be used as a starting point for investigating landscapes of k-noncrossing RNA structures.

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