

Properties of RNA secondary structure matching models

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RNA secondary structures have been modeled using a variety of matching families. We first explore the intersections of different matching families which are models for likely RNA secondary structures. We then introduce their respective enumeration sequences and prove our proposed equations for enumeration. Next, we prove a formula for the number of matchings with a given crossing number for a variety of matching families. Then we develop a new statistic called the pseudoknot number and find the maximum pseudoknot number on a given set of matchings. We end by providing a comparison between the crossing number, nesting number, and pseudoknot number for three matching families on nine edges.

1. Introduction

1A. *Background Information.* Ribonucleic acid (RNA) is an important molecule in all living organisms that directly codes for amino acids and acts as a messenger between DNA and ribosomes to make proteins. RNA is a single-stranded molecule made up of the nucleotides adenine, guanine, cytosine, and uracil. This string of nucleotides folds over on itself and forms secondary bonds between some of its nucleotides [Martinez and Riehl 2017]. Biologists and mathematicians have spent a great deal of time studying these RNA secondary structures [Condon et al. 2004; Jefferson 2015]. In mathematics we represent the secondary structures using a type of graph called a matching. A matching is a graph-theoretical structure in which each vertex has at most degree 1. In our matchings each vertex represents a nucleotide and each edge represents a secondary bond. Since RNA is a string of ordered nucleotides connected by bonds, we list all the vertices of the matching in order along a horizontal line (the backbone) where the edges connect above the vertices. To simplify the graph, we omit any nucleotides that are not part of a

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Figure 1. An RNA motif (top) [Ronan 2006] and its matching (bottom).

secondary bond, making each matching a complete matching on 2n vertices and n edges. In a complete matching, sometimes called a perfect matching, every vertex is incident to one edge. To recreate an RNA structure with isolated vertices from its matching we can add them into the complete matching in their corresponding spots. Figure 1 demonstrates an RNA motif represented as a matching.

For an edge, *i*, in a matching, we write $i = (i_1, i_2)$, where i_1, i_2 are the positions of the left- and right-endpoints of the edge, respectively. A pair of edges $i = (i_1, i_2)$ and $j = (j_1, j_2)$ in a matching, *M*, are said to be crossing if $i_1 < j_1 < i_2 < j_2$. A pair of edges are said to be nested if $i_1 < j_1 < j_2 < i_2$. Similarly, if $j_1 = i_1 + 1$ and $j_2 = i_2 + 1$, then *i* and *j* form a hairpin. Finally, a nested sequence of *n* edges is called a ladder [Martinez and Riehl 2017]. In Section 4 we will be particularly interested in examining pseudoknot numbers for certain matching families along with all perfect matchings.

A number of statistics can be applied to the matchings (e.g., crossing number and nesting number). The crossing number, cr(M), counts the number of times a pair of edges in the matching cross. The nesting number for one edge counts the number of edges nested under said edge. The nesting number statistic for a matching, ne(M), is the sum of the nesting numbers for each edge in the matching.

We introduce here a biologically motivated statistic called the pseudoknot number, pknot(M). A pseudoknot occurs in a strand of RNA when the strand folds on itself and forms secondary bonds between nucleotides, and then the same strand wraps around and forms secondary bonds again. See Figure 1 for an example. These formations are important because viruses have pseudoknots to infiltrate a host cell



Figure 2. A matching on four edges that can be represented as the permutation $\sigma = 17253468$.

to cause such diseases as hepatitis C, HIV, and SARS [Brierley et al. 2007]. The pseudoknot number of a matching, pknot(M), counts the number of pseudoknots on the RNA motif by deflating any ladders in the matching and then finding the crossing number on the resulting matching.

Matchings can also be represented as permutations of length 2n. The permutation is constructed by numbering the vertices (i.e., the nucleotides along the backbone) from 1 to 2n. We then work from left to right recording the left vertex number followed by the right vertex number of each edge that we encounter. This creates a permutation in which the odd indices are monotonically increasing. For example, the matching in Figure 2, written as a permutation, is 17253468. We represented matchings as permutations in our code that generated data and helped us arrive at conjectures.

Definition 1.1. The *Catalan numbers* are a sequence that appears in mathematics in many different settings. This sequence is enumerated by the formula

$$C_n = \frac{2n}{(n+1)!\,n!},$$

where C_n represents the *n*-th Catalan number. This sequence begins

1, 2, 5, 14, 132,

Example 1.1. Given *n* pairs of parentheses, there are C_n many ways to arrange these parentheses such that every open parenthesis has a matching closed parenthesis after it. Table 1 shows the ways to arrange *n* pairs of parentheses where $1 \le n \le 4$.

There is clear bijection between these *n* pairs of parentheses and the noncrossing matchings on *n* edges. A left parenthesis corresponds to where an edge starts and a right parenthesis corresponds to where an edge ends. For example, Figure 3 corresponds to the arrangement of five pairs of parentheses given by ()(()())().

Therefore, it is known that the Catalan numbers also count the noncrossing matchings.

In Section 1B we briefly describe families of matchings that represent RNA secondary structures where unlikely biological structures are significantly restricted. Many of these families of matchings are inductively built starting from a single

n	arrangements	no. of arrang.
1	0	1
2	()(), (())	2
3	000, 0(0), (0)0, (00), ((0))	5
4	0000, (0)00, 0(0)0, 00(0), 0(00),	14
	(())(()), (()())(), ((()))(), ()(())), (()()), ()()), ()()), ()()), ()()()), ()), ()), ()()), ()()), ())), ())), ())), ())), ())), ())))))))	
	((())()), (()(())), ((()())), (((())))	

Table 1. The Catalan-many ways to arrange *n* pairs of parentheses, where $1 \le n \le 4$ [Davis 2016].



Figure 3. The matching corresponding to the arrangement of five pairs of parentheses given by ()(()())().

edge or a hairpin. Algebraic generating functions for the five main families of matchings have been found [Jefferson 2015]. In Sections 2 and 3 we will investigate intersections of these families.

1B. *Hairpin-only Families.* Mathematical biologists have defined five hairpinonly families of matchings that model RNA secondary structures. These families (often named after the people who first studied them) are: LHF (largest hairpin family), D&P (Dirks and Pierce), R&G (Rieder and Giegerich), C&C (Cao and Chen), and L&P (Lyngsø and Pedersen) (shown in Figure 4 from least restrictive to most restrictive) [Jefferson 2015].

Suppose we have two matchings M and N with 2m and 2n vertices respectively. For a vertex i in M, the vertex insertion in M by N after i is the matching with



Figure 4. The inclusions among hairpin-only families.



Figure 5. A hairpin with the left edge inflated by a hairpin.

2m+2n vertices in which a copy of N is inserted between i and i+1 in M [Jefferson 2015]. Now, given any matching Q with q edges and a matching R with r edges, if (i, j) is an edge of Q then the *edge inflation of Q by R* at (i, j) is the matching on the vertices 2q + 2r - 2 in which the vertex i is replaced by the left-endpoints of R, the vertex j is replaced by the right-endpoints of R, and the edges between these two sets of vertices are defined as they are in R [Jefferson 2015]. An example of edge inflation by a matching is shown in Figure 5.

LHF matchings. The *largest hairpin family* is formed by matchings that begin with either a single edge or a hairpin. Then arbitrary vertex insertions and edge inflations by matchings may be performed.

An example of a matching in LHF is shown on the right-hand side of Figure 5. To construct this matching we start with a hairpin and inflate one of its edges by another hairpin.

The D&P (Dirks and Pierce) family. The D&P family can be constructed inductively by beginning with either a single edge or a hairpin. Then the following procedures can be performed: (1) inflate an edge by a ladder and (2) insert one D&P matching into another. The D&P family differs from LHF because instead of being closed under edge inflation, only edge inflations by ladders are allowed. An example of a D&P matching is shown in Figure 6. To construct this matching we start with a hairpin and then inflate its left edge by a ladder. Then we insert a hairpin between the two edges of the ladder.

The R&G (Rieder and Giegerich) family. Starting from either a single edge or a hairpin, matchings of the R&G family can be built inductively via the following operations: (1) insert R&G matchings into the places shown in Figure 7, followed by (2) inflating the original edge(s) by ladders. An example of an R&G matching is shown in Figure 8. To construct this matching we start with a hairpin and insert another hairpin into the middle.



Figure 6. A D&P matching on five edges.



Figure 7. The allowable places for insertion in the R&G family.



Figure 8. An R&G matching on four edges.

The C&C (Cao and Chen) family. Starting from either a single edge or a hairpin, matchings of the *C&C family* can be built inductively via the following operations: (1) insert C&C matchings in the allowable places (as shown in Figure 9) and then (2) inflate the original edge(s) by ladders. An example of a C&C matching is shown in Figure 10. To construct this matching we start with a single edge and insert a hairpin under the edge.

The L&P (Lyngsø and Pedersen) family. Starting from either a single edge or a hairpin, the matchings of the L&P family can be built inductively via the following operations: (1) inflate an edge of an L&P matching by a ladder and (2) insert a noncrossing matching into an L&P matching. An example of an L&P matching is shown in Figure 11. To construct this matching we start with a hairpin and insert a noncrossing matching of size 2 into the middle of the hairpin.

We studied different intersections of the hairpin-only families. The Venn diagram in Figure 12 depicts the different intersections in which we have labeled each distinct region using script letters. For example, A is the group of matchings that are both L&P and C&C. B is the group of matchings that are L&P and R&G but not C&C. In Sections 2 and 3 we will describe A and B and the formulae that enumerate these matchings. In Section 4 we will examine the crossing number, nesting number, and



Figure 9. The allowable places for insertion in the C&C family.



Figure 10. A C&C matching on three edges.



Figure 11. An L&P matching on four edges.



Figure 12. The Venn diagram that shows the different regions we have analyzed.

pseudoknot number statistics on L&P matchings, C&C matchings, and all perfect matchings. We will then compare the distributions of these statistics for each of the given families on nine edges.

2. Matchings that are L&P and C&C (i.e., in A)

Matchings in A must be both L&P and C&C matchings. Figure 13 shows all 11 matchings in A with three edges.

For a small *n*, where *n* is the number of edges in each matching, the sequence of matchings in A starting at n = 1 is given by, see [Goryl 2017b],

$$1, 3, 11, 39, 134, 456, 1557, 5364, \dots$$
(1)



Figure 13. The 11 matchings in A with three edges.



Figure 14. Matching in A with nine edges.

The matchings that are both L&P and C&C can be created inductively through the following operations in the given order:

- We begin with either a single edge or a hairpin.
- We can insert noncrossing matchings, to ensure the matching is L&P, into the insertion spots as shown in Figure 10, to ensure the matching is C&C.
- Finally, we can inflate the original edge(s) by ladders. Inflating the original edges last ensures that the matchings are C&C as we cannot insert matchings between ladders.

Each matching in \mathcal{A} can be split into two separate parts: a (possibly empty) noncrossing matching and a (possibly empty) hairpin first matching. Let \mathcal{NCM}_n be the noncrossing matchings on *n* edges and let NCM_n = $|\mathcal{NCM}_n|$. Let \mathcal{HF}_n be the matchings in \mathcal{A}_n whose leftmost edge is part of a hairpin and let HF_n = $|\mathcal{HF}_n|$.

For example, in Figure 14, the leftmost edge is part of a noncrossing matching consisting of three edges, so these three edges are in \mathcal{NCM}_3 . The next part of the matching has its leftmost edge as part of a hairpin. So these six edges are in \mathcal{HF}_6 .

Lemma 2.1. The number of ways to insert (possibly empty) noncrossing matches into three possible positions with m total edges is $C_{m+2} - C_{m+1}$.

Proof. Since the edges we insert are noncrossing and the noncrossing matchings are counted by the Catalan numbers, the summation of these products of three Catalan numbers with subscripts i, j, k would enumerate the number of ways we could insert a total of m edges, made of noncrossing matchings. It can be proved using generating functions [Sloane 2010b] for this sequence that

$$\sum_{\substack{i,j,k \ge 0 \\ i+j+k=m}} C_i C_j C_k = C_{m+2} - C_{m+1}.$$

Lemma 2.2. *Matchings in A where the leftmost edge is part of the hairpin can be enumerated by the formula*

$$HF_n = \sum_{j=1}^n C_j - n.$$

Proof. Consider matchings in A where the leftmost edge is part of a hairpin. Since these matchings are C&C, there are only three insertion spots, and n - 2 edges left

to insert. By Lemma 2.1, there are $C_n - C_{n-1}$ ways to do so. If we have either side inflated by one ladder, it can either inflate the left or right side of the hairpin, and then we have n-3 edges left to insert, so that's $2(C_{n-1} - C_{n-2})$ more matchings. If we continue on with this process, the number of ways to insert noncrossing matchings into a hairpin, now taking ladders into consideration, is given by

$$(C_n - C_{n-1}) + 2(C_{n-1} - C_{n-2}) + 3(C_{n-2} - C_{n-3}) + \dots + (n-1)(C_2 - C_1)$$

= $C_n - C_{n-1} + 2C_{n-1} - 2C_{n-2} + 3C_{n-2} - 3C_{n-3} + \dots + (n-1)C_2 - (n-1)C_1$
= $C_n + C_{n-1} + C_{n-2} + \dots + C_3 + C_2 - (n-1)$ since $C_1 = 1$.

In order to sum over all the Catalan numbers, we can add in C_1 and then subtract $C_1 = 1$ at the end, giving us

$$\sum_{j=1}^{n} C_j - n.$$

Lemma 2.3. All matchings in A can be enumerated by

$$\sum_{i=0}^{n} C_i \operatorname{HF}_{n-i}$$

with initial conditions

 $HF_0 = 1$, $HF_1 = 0$, $HF_2 = 1$, $C_0 = 1$, $C_1 = 1$,

where C_i are the Catalan numbers, and HF_n represents the number of matchings that are both L&P, C&C, and have the leftmost edge as part of a hairpin.

Proof. Matchings in A are completely described by all combinations of NCM_{*i*} and HF_{*n*-*i*}. Since we know that the Catalan numbers enumerate the noncrossing matchings, by [Sloane 2010a] we know all matchings in A are enumerated by

$$\sum_{i=0}^{n} C_i \operatorname{HF}_{n-i}.$$

Theorem 2.1. *The matchings that are both L&P and C&C can be enumerated by the formula*

$$\sum_{i=0}^{n-2} C_i \left(\sum_{j=1}^{n-i} C_j - (n-i) \right) + C_n,$$

where C_k is the k-th Catalan number.

Proof. From Lemma 2.3 we know the first sum will be

$$\sum_{i=0}^{n} C_i \operatorname{HF}_{n-i}.$$

266 N. ANDERSON, M. BREUNIG, K. GORYL, H. LEWIS, M. RIEHL AND M. SCANLAN

Combining this with Lemma 2.2, we see that

$$|\mathcal{A}| = \sum_{i=0}^{n-2} C_i \left(\sum_{j=1}^{n-i} C_j - (n-i) \right) + C_n.$$

Example 2.1. Suppose we want to determine the number of matchings that are L&P and C&C with three edges.

Let n = 3. So,

$$\sum_{i=0}^{n-2} C_i \left(\sum_{j=1}^{n-i} C_j - (n-i) \right) + C_n = \sum_{i=0}^{1} C_i \left(\sum_{j=1}^{3-i} C_j - (3-i) \right) + C_3$$
$$= C_0 \left(\sum_{j=1}^{3} C_j - 3 \right) + C_1 \left(\sum_{j=1}^{2} C_j - 2 \right) + C_3$$
$$= C_0 (C_1 + C_2 + C_3 - 3) + C_1 (C_1 + C_2 - 2) + C_3$$
$$= 1(1+2+5-3) + 1(1+2-2) + 5 = 11,$$

which agrees with formula (1). The 11 matchings with three edges that are L&P and C&C are shown in Figure 13.

3. Matchings that are L&P and R&G but not C&C (i.e., in B)

Matchings in \mathcal{B} must be both L&P and R&G but not C&C. Figure 15 shows all eight matchings in \mathcal{B} with four edges.



Figure 15. The eight matchings in \mathcal{B} with 4 edges.



Figure 16. The smallest matching in \mathcal{B} .

For a small *n*, where *n* is the number of edges in each matching, the sequence of matchings in \mathcal{B} starting at *n* = 1 is given by, see [Goryl 2017a],

$$0, 0, 1, 8, 42, 186, 759, 2970, 11369, \dots$$
 (2)

The group of matchings that are L&P and R&G but not C&C can be created inductively through the following operations in the given order:

- We must begin with a hairpin that has a single edge inserted into the middle of the hairpin as shown in Figure 16. The edge inserted into the middle of the hairpin will ensure that all matchings are not C&C.
- To ensure that the matchings are L&P, we next insert noncrossing matchings.
- Finally, we can inflate the edges of the hairpin by ladders. Inflating the edges of the hairpin last ensures that the matchings are R&G, in which you cannot insert matchings between ladders.

Lemma 3.1. Let a_n be the number of matchings in \mathcal{B} with n edges where the last step in its inductive creation is inflation by a ladder, denoted by inflate(n). Then $a_n = 2a_{n-1} - a_{n-2}$.

Proof. In order for a matching to be R&G, inflations of the original edges must occur after all insertions. Since matchings in \mathcal{B} start with a hairpin, the only edges we can inflate are the two edges that make up the hairpin. To obtain these matchings with n edges, we can take all matchings in \mathcal{B} with n - 1 edges and inflate each matching's left edge of the hairpin by a ladder. That gives us a_{n-1} matchings. Then, for the matchings in \mathcal{B} with n - 1 edges, we can inflate each matching's right edge of the hairpin by a ladder, we can inflate each matching. In total, this gives us $2a_{n-1}$ matchings, but we have over-counted. Inflating the left side of the hairpin and then the right is the same as inflating the right side of the hairpin and then the left, so we want to remove those matchings with n - 2 edges in \mathcal{B} and inflate the left edge of the hairpin by one ladder and then right edge of the hairpin by one ladder and then right edge of the hairpin by one ladder and then right edge of the hairpin by one ladder and then right edge of the hairpin by one ladder and then right edge of the hairpin by one ladder, we get a_{n-2} matchings with n edges. So, if we subtract the over-counted matchings, we get $2a_{n-1} - a_{n-2}$ matchings in inflate(n).

Lemma 3.2. *Matchings with n edges in* \mathcal{B} *where the last step is an insertion, denoted by* ins(n)*, are enumerated by*

$$\frac{6}{n+3}\binom{2n-1}{n-3}.$$
(3)



Figure 17. Five allowable places for insertion in \mathcal{B} .

Proof. Starting with a hairpin, we can insert noncrossing matchings into the five different insertion spots shown in Figure 17 given there is at least one element of NCM₁ in the middle of the hairpin. We know that the inserted noncrossing matchings cannot be inserted between ladders because the matchings must be both R&G and L&P. Note, for R&G matchings there are only four insertion spots because we cannot insert to the left of the hairpin. Noncrossing matchings inserted on the left of the hairpin can be thought of as starting with a noncrossing matching and inserting a matching containing a hairpin on the right. Therefore, we will be inserting noncrossing matchings into five insertion spots. Letting *i*, *j*, $k \ge 1$, we insert *i* - 1 edges on the left side of the hairpin, *j* edges in the middle of the hairpin (since we must have at least one edge inserted here), and k - 1 edges on the right side of the hairpin. Since there are already two edges included in the hairpin, i - 1 + j + k - 1 = n - 2, which implies i + j + k = n.

First, consider noncrossing matchings that are on the left side of the hairpin. This includes both matchings that are on the far left outside of the hairpin and matchings that are under the left edge of the hairpin. There are $C_{i-1}C_0 + C_{i-2}C_1 + \cdots + C_1C_{i-2} + C_0C_{n-1}$ ways to insert i-1 edges into two insertion spots on the left side of the hairpin. It is known that sum is equal to C_i [Davis 2016]. Therefore, there are C_i ways to insert i-1 edges into the left side of the hairpin. Likewise, there are C_k ways to insert k-1 edges into the right side of the hairpin, which includes on the far right outside of the hairpin and matchings under the right edge of the hairpin. There are C_j ways to insert j edges into the middle of a hairpin because we can only insert noncrossing matchings. This implies we can enumerate matchings in ins(n) by

$$\sum_{\substack{i,j,k\geq 1\\i+j+k=n}} C_i C_j C_k$$

It is known this is given by the closed form (3) [Sloane 1991].

Theorem 3.1. *The matchings that are L&P and R&G but not C&C can be enumerated by the formula*

$$a_n = 2a_{n-1} - a_{n-2} + \frac{6}{n+3} \binom{2n-1}{n-3}.$$
(4)

Proof. Since we inductively build matchings in \mathcal{B} with exactly two operations, Lemmas 3.1 and 3.2 completely describe how to build all matchings in \mathcal{B} . Therefore, by Lemmas 3.1 and 3.2, we can add our two formulas together to obtain the recurrence relation (4), which enumerates all matchings in \mathcal{B} .

This recurrence relation has no closed formula, although it can be written using hypergeometric series. Since there is a closed form for L&P matchings and we have now found equations for A and B, we can use these to enumerate matchings in C using subtraction.

Example 3.1. Suppose we want to find the matchings in \mathcal{B} with n = 4 edges. Then we can compute

$$a_4 = 2a_3 - a_2 + \frac{6}{7}\binom{7}{1} = 2(1) - 0 + 7\frac{6}{7} = 8,$$

which agrees with formula (2). The eight matchings with four edges in \mathcal{B} can be found in Figure 15.

4. Statistics

We implemented the following statistics and constructions of each hairpin family in Python, and those programs are available upon request.

4A. *L&P Matchings.* L&P matchings insert only noncrossing matchings; therefore the only way to have two crossing edges is to begin with a hairpin. The only way to increase the crossing number is to inflate the edges of the hairpin. Because all of the crossings happen in the hairpin, we can count the number of crossings by taking the product of the number of edges that inflate the left side of the hairpin and the number of edges that inflate the right side of the hairpin.

Theorem 4.1. The number of L&P matchings on n edges with a given crossing number h > 0 is 2F+1

$$\sum_{\substack{(\gamma_1, \gamma_2, \dots, \gamma_k) \ (\alpha_1, \alpha_2, \dots, \alpha_{(2E+1)}) \\ \gamma_i \ge 0 \\ \gamma_i \le \beta_i \forall i}} \sum_{\substack{\alpha_i \ge 0 \\ \sum \alpha_i = n-E}} \prod_{i=1}^{2E+1} C_{\alpha_i}$$

where $h = p_1^{\beta_1} p_2^{\beta_2} \cdots p_k^{\beta_k}$ is the prime factorization of h, $p_1^{\gamma_1} p_2^{\gamma_2} \cdots p_k^{\gamma_k}$ is a factor of h, and E is $p_1^{\gamma_1} p_2^{\gamma_2} \cdots p_k^{\gamma_k} + p_1^{\beta_1 - \gamma_1} p_2^{\beta_2 - \gamma_2} \cdots p_k^{\beta_k - \gamma_k}$.

Proof. Let *h* be the desired crossing number and *n* be the number of edges in the L&P matching. Because h > 0 and the matchings are L&P we know that there is exactly 1 hairpin in the matching. Then let $h = p_1^{\beta_1} p_2^{\beta_2} \cdots p_k^{\beta_k}$ be its unique prime factorization. Each factor of *h* is then given by $p_1^{\gamma_1} p_2^{\gamma_2} \cdots p_k^{\gamma_k}$ with $0 \le \gamma_i \le \beta_i$. The product of the edges on the right and the left sides of the hairpin must be *h* so there must be $p_1^{\gamma_1} p_2^{\gamma_2} \cdots p_k^{\gamma_k}$ edges on the left side of the hairpin and $p_1^{\beta_1-\gamma_1} p_2^{\beta_2-\gamma_2} \cdots p_k^{\beta_k-\gamma_k}$ edges on the right side of the hairpin. Then there are n - E edges left to insert into the matching in some of 2E + 1 places. Then consider the number of noncrossing edges inserted into each spot of the matching as a vector $\vec{\alpha}$. If each α_i will be the number of edges inserted into the *i*-th spot of

270 N. ANDERSON, M. BREUNIG, K. GORYL, H. LEWIS, M. RIEHL AND M. SCANLAN



Figure 18. Places to insert in an L&P matching.

the matching, the insertion vector $\vec{\alpha}$ is given by $(\alpha_1, \alpha_2, \dots, \alpha_{2E+1})$, where $\alpha_i \ge 0$ and $\sum_i \alpha_i = n - E$. The insertions must be noncrossing because the matchings are L&P; therefore there are Catalan-many ways to insert each noncrossing matching. Then there are $C_{\alpha_1}C_{\alpha_2}\cdots C_{\alpha_{2E+1}}$ ways to insert each $\vec{\alpha}$ into the matching. We can sum over all $\vec{\alpha}$ to find all the matchings with the given number of edges on the left and right sides of the hairpin. Then we sum over all the possible factors of *h* to get all possible L&P matchings on *n* edges with crossing number *h*.

For example, to find the number of L&P matchings on n = 9 edges with a crossing number of h = 6 we will start by writing the prime factorization of h: $h = 2^1 * 3^1$. Using the prime factorization we can find all of the factors of h: 1, 2, 3, 6. We begin with our first factor, 1, being the number of edges on the left side of the hairpin. We know the product of the number of edges on the left and right sides of the hairpin must be 6, so there must be six edges on the right side of the hairpin. Then there are a total of seven edges in the hairpin, and there are two edges left to insert into the matching in the 15 places shown by the arrows in Figure 18. There are two edges left to insert into the inflated hairpin and they could be inserted into the same place or into two different places. If they are inserted into two different places the corresponding $\vec{\alpha}$ would contain two 1's, and 13 0's. There are $\binom{15}{2}$ distinct $\vec{\alpha}$ of this type. There are C_1 ways to arrange the first inserted edge and there are C_1 ways to arrange the second inserted edge. If both edges are inserted into the same place the corresponding $\vec{\alpha}$ would contain one 2 and 14 0's. There are 15 distinct $\vec{\alpha}$ of this type. There are C_2 ways to arrange the inserted noncrossing matching of size 2. The number of L&P matchings on nine edges with one edge on the left side of the hairpin and six edges on the right side of the hairpin is therefore $\binom{15}{2}C_1C_1+15C_2=135$. We repeat this process with each remaining factors of h, 2, 3, and 6, where each factor is the number of edges on the left side of the hairpin. After considering all factors we find that there are 4758 L&P matchings on nine edges with a crossing number of six.

Example 4.1. Suppose we want to find the number of L&P matchings with n = 4 edges and h = 1.

We start with the prime factorization of h: h = 1. Thus, the only factor of h is 1. This means there is one edge on each of the left and right sides of the hairpin. Hence,



Figure 19. The 20 matchings that are L&P with n = 4 edges and h = 1.

there are two edges left to insert into five spots. Using the same process as before, we get $\binom{5}{2}C_1C_1 + 5C_2 = 20$ matchings. These 20 matchings are found in Figure 19.

4A1. *Maximum values.* To find the maximum crossing number of an L&P matching on *n* edges, we require that all edges be part of the initial hairpin and that there be as close to an equal number edges inflated on each side of the hairpin as possible. This results in a maximum crossing number of $\frac{1}{8}(2n^2 - 1 + (-1)^n)$, which is the closed form of $\sum \lfloor \frac{1}{2}n \rfloor + 1$, which is obtained by successively adding one edge to the previously maximally inflated hairpin. We note that the formula in Theorem 4.1 is zero if $h > \sum \lfloor \frac{1}{2}n + 1 \rfloor$.

The maximum nesting number of an L&P matching is the same as that of a noncrossing matching (i.e., a ladder on *n* edges), which is $\frac{1}{2}n(n+1)$.

4B. *C&C.* The maximum crossing and nesting number of a C&C matching of n edges is the same as that of an L&P matching. This is because the C&C matchings contain the noncrossing matchings (i.e., the maximally nested matchings) and the matchings with the maximum crossing number are L&P and C&C.

4C. A, matchings that are L&P and C&C.

Lemma 4.1. If a C&C matching that contains exactly one hairpin is inserted to the right of a noncrossing matching, the obtained matching is C&C.

271

272 N. ANDERSON, M. BREUNIG, K. GORYL, H. LEWIS, M. RIEHL AND M. SCANLAN



Figure 20. Allowable insertion spots for A.

Proof. A noncrossing matching is C&C, and according to the inductive definition of C&C matchings we can insert another C&C matching to the right of it. \Box

Lemma 4.2. There are four places to insert noncrossing matchings in a hairpin to obtain a matching in A. Matchings cannot be inserted between ladders of the hairpin, and they cannot be inserted into the middle of the hairpin.

Proof. By Lemma 4.1 if we insert a noncrossing matching to the far left of a C&C matching that contains exactly one possibly inflated hairpin, the obtained matching is C&C. By the rules of creating C&C matchings, if we insert a noncrossing matching into the spots shown by the three remaining arrows in Figure 20 it will still be C&C. We cannot insert noncrossing matchings in between ladders or in the middle of the hairpin because then it would no longer be C&C. Because there is only one possibly inflated hairpin and we are inserting only noncrossing matchings we are guaranteed that these matchings are also L&P, and therefore they are in \mathcal{A} .

Theorem 4.2. The number of matchings in A on n edges with crossing number h > 0 is given by

$$\sum_{\substack{(\gamma_1, \gamma_2, \dots, \gamma_k) \ (\alpha_1, \alpha_2, \alpha_3, \alpha_4) \\ \gamma_i \geq 0 \\ \gamma_i \leq \beta_i \forall i}} \sum_{\substack{\alpha_i \geq 0 \\ \sum \alpha_i = n - E}} \prod_{i=1}^{\tau} C_{\alpha_i},$$

where $h = p_1^{\beta_1} p_2^{\beta_2} \cdots p_k^{\beta_k}$ is the prime factorization of h, $p_1^{\gamma_1} p_2^{\gamma_2} \cdots p_k^{\gamma_k}$ is a factor of h, and E is $p_1^{\gamma_1} p_2^{\gamma_2} \cdots p_k^{\gamma_k} + p_1^{\beta_1 - \gamma_1} p_2^{\beta_2 - \gamma_2} \cdots p_k^{\beta_k - \gamma_k}$.

Proof. Let *h* be the given crossing number and *n* be the number of edges in the matching in *A*. Because h > 0 and the matchings are L&P we know that there is exactly one possibly inflated hairpin in the matching. Then let $h = p_1^{\beta_1} p_2^{\beta_2} \cdots p_k^{\beta_k}$ be its unique prime factorization. Each factor of *h* is then given by $p_1^{\gamma_1} p_2^{\gamma_2} \cdots p_k^{\gamma_k}$. Since these matchings are L&P, the product of the edges on the right and the left sides of the hairpin must be *h*. Thus, there must be $p_1^{\gamma_1} p_2^{\gamma_2} \cdots p_k^{\gamma_k}$ edges on the left side of the hairpin and $p_1^{\beta_1-\gamma_1} p_2^{\beta_2-\gamma_2} \cdots p_k^{\beta_k-\gamma_k}$ edges on the right side of the hairpin. Then the total number of edges *E* in the hairpin is given by $p_1^{\gamma_1} p_2^{\gamma_2} \cdots p_k^{\gamma_k} + p_1^{\beta_1-\gamma_1} p_2^{\beta_2-\gamma_2} \cdots p_k^{\beta_k-\gamma_k}$. Then there are n - E edges left to insert into the matching. By Lemma 4.2 there are four places to insert. The insertions must be noncrossing because the matchings are L&P; therefore there are Catalan-many ways to insert



Figure 21. The 14 matchings in A with n = 4 edges and h = 1.

each noncrossing matching. If we think about the number of noncrossing edges inserted into each spot of the matching as a vector $\vec{\alpha}$ then each α_i will be the number of edges inserted into the *i*-th spot of the matching. The insertion vector $\vec{\alpha}$ is given by $(\alpha_1, \alpha_2, \alpha_3, \alpha_4)$, where $\alpha_i \ge 0$ and $\sum_i \alpha_i = n - E$. Then there are $C_{\alpha_1}C_{\alpha_2}C_{\alpha_3}C_{\alpha_4}$ ways to insert each $\vec{\alpha}$ into the matching. We can then sum over all $\vec{\alpha}$ to find all the matchings with the given number of edges on the left and right sides of the hairpin. Then we sum over all the possible factors of *h* to get all possible matchings in \mathcal{A} on *n* edges with crossing number *h*.

Example 4.2. Suppose we want to find the number of matchings in A with n = 4 edges and h = 1.

We start with the prime factorization of h: h = 1. Thus, the only factor of h is 1. This means there is one edge on each of the left and right sides of the hairpin. Hence, there are two edges left to insert into four spots. Using the same process as before, we get $\binom{4}{2}C_1C_1 + 4C_2 = 14$ matchings. These 14 matchings are found in Figure 21.

4D. B, matchings that are R&G and L&P but not C&C.

Lemma 4.3. There are six places to insert noncrossing matchings in an inflated hairpin that has one edge inserted into the middle in order for a matching in B. These places are shown in Figure 22.

Proof. By Lemma 4.1 if we insert a noncrossing matching to the far left of a C&C matching that contains exactly one hairpin, the obtained matching is C&C. Therefore if we insert a noncrossing matching to the far left of an R&G matching that contains exactly one hairpin, then the obtained matching is R&G. We can't insert matchings between the ladders that inflate the hairpin because then the matching would not



Figure 22. Allowable insertion spots for \mathcal{B} .

be R&G. The obtained matching is also L&P because it has exactly one hairpin, and only noncrossing matchings are inserted. The obtained matching is not C&C because of the guaranteed single edge inserted into the middle of the hairpin. We don't insert to the left of the single edge in the middle of the hairpin in order to prevent duplicates from being made.

Theorem 4.3. The number of matchings in \mathcal{B} on n edges with crossing number h > 0 is given by the formula

$$\sum_{\substack{(\gamma_1,\gamma_2,...,\gamma_k)\\ \gamma_i \ge 0\\ \gamma_i \le \beta_i \forall i}} \sum_{\substack{(\alpha_1,\alpha_2,...,\alpha_6)\\ \alpha_i \ge 0\\ \sum \alpha_i = n-E-1}} \prod_{i=1}^6 C_{\alpha_i},$$

where $h = p_1^{\beta_1} p_2^{\beta_2} \cdots p_k^{\beta_k}$ is the prime factorization of h, $p_1^{\gamma_1} p_2^{\gamma_2} \cdots p_k^{\gamma_k}$ is a factor of h, and E is $p_1^{\gamma_1} p_2^{\gamma_2} \cdots p_k^{\gamma_k} + p_1^{\beta_1 - \gamma_1} p_2^{\beta_2 - \gamma_2} \cdots p_k^{\beta_k - \gamma_k}$.

Proof. Let h be the given crossing number and n be the number of edges in the matching in \mathcal{B} . Because h > 0 and the matchings are L&P we know that there is exactly one possibly inflated hairpin in the matching. Then let $h = p_1^{\beta_1} p_2^{\beta_2} \cdots p_k^{\beta_k}$ be its unique prime factorization. Each factor of *h* is then given by $p_1^{\gamma_1} p_2^{\gamma_2} \cdots p_k^{\gamma_k}$. Since these matchings are L&P, the product of the edges on the right and the left sides of the hairpin must be *h*. Thus, there must be $p_1^{\gamma_1} p_2^{\gamma_2} \cdots p_k^{\gamma_k}$ edges on the left side of the hairpin and $p_1^{\beta_1 - \gamma_1} p_2^{\beta_2 - \gamma_2} \cdots p_k^{\beta_k - \gamma_k}$ edges on the right side of the hairpin. Then the total number of edges *E* in the hairpin is given by $p_1^{\gamma_1} p_2^{\gamma_2} \cdots p_k^{\gamma_k} + p_1^{\beta_1 - \gamma_1} p_2^{\beta_2 - \gamma_2} \cdots p_k^{\beta_k - \gamma_k}$. Then there are n - E - 1 edges left to insert into the matching. We subtract 1 since a single edge is guaranteed to be inserted into the middle of the hairpin. By Lemma 4.3 there are six places to insert. The insertions must be noncrossing because the matchings are L&P. Therefore there are Catalanmany ways to insert each noncrossing matching. If we think about the number of noncrossing edges inserted into each spot of the matching as a vector $\vec{\alpha}$, then each α_i will be the number of edges inserted into the *i*-th spot of the matching. The insertion vector $\vec{\alpha}$ is given by $(\alpha_1, \alpha_2, \dots, \alpha_6)$, where $\alpha_i \ge 0$ and $\sum_i \alpha_i = n - E - 1$. Then there are $C_{\alpha_1}C_{\alpha_2}\cdots C_{\alpha_6}$ ways to insert each $\vec{\alpha}$ into the matching. We can then sum over all $\vec{\alpha}$ to find all the matchings with the given number of edges on the left and right sides of the hairpin. Then we sum over all the possible factors of h to get all possible matchings in \mathcal{B} on *n* edges with crossing number *h*.



Figure 23. The 27 matchings in \mathcal{B} with n = 5 edges and h = 1.

Example 4.3. Suppose we want to find the number of matchings in \mathcal{B} with n = 5 edges and h = 1.

We start with the prime factorization of h: h = 1. Thus, the only factor of h is 1. This means there is one edge on each of the left and right sides of the hairpin. Hence, there are two edges left to insert into four spots. Using the same process as before, we get $\binom{6}{2}C_1C_1 + 6C_2 = 27$ matchings. These 27 matchings are found in Figure 23.

4E. *Maximum Pseudoknot.* The pseudoknot number of a matching is found by deflating the ladders of every edge in the matching and finding the crossing number of the new matching. To find the maximum pseudoknot number of a matching on n edges, we want a matching that has the highest crossing number once its edges have been deflated.

Let M_n be the set of all perfect matchings on n edges. Let CC_n be the set of all C&C matchings on n edges. For a set of matchings A, let $pknot_{max}(A) = max\{pknot(M) \mid M \in A\}$.



Figure 24. Matching that gives the maximum pseudoknot number on four edges for the C&C family.

Definition 4.1. We define a deflation as follows. If we have two edges $i = (i_1, i_2)$ and $j = (j_1, j_2)$ such that $i_1 = j_1 - 1$ and $i_2 = j_2 + 1$, then we delete edge *i*.

Theorem 4.4. The maximum pseudoknot number of the set of C&C matchings on *n* edges is given by

$$pknot_{max}(CC_n) = \begin{cases} \frac{1}{2}n, & n \in \mathbb{N} \text{ and is even} \\ \frac{1}{2}(n-1), & n \in \mathbb{N} \text{ and is odd.} \end{cases}$$

Proof. In C&C matchings, the maximum pseudoknot number occurs when we maximize the number of noninflated hairpins since we cannot insert between ladders in C&C matchings.

<u>Case 1</u>: *n* is even. Since *n* is even, every two edges must be involved in distinct hairpins in the matching in order to maximize the number of noninflated hairpins. Then every matching must have $\frac{1}{2}n$ hairpins. Because our matching *M* consists of strictly hairpins, there are no deflations. Hence, pknot(*M*) = cr(*M*). Since all the hairpins are not inflated, to find cr(*M*) we can count the number of hairpins. Thus cr(*M*) = $\frac{1}{2}n$ = pknot_{max}(CC_n).

<u>Case 2</u>: *n* is odd. When *n* is odd, every two edges except for one must be involved in distinct hairpins in order to maximize the number of noninflated hairpins. Then the matching *M* must have $\frac{1}{2}(n-1)$ hairpins. Whether the final edge not involved in a hairpin is inserted or inflates another edge has no effect on the pseudoknot number. After deflations on all edges are made, there are still guaranteed to be $\frac{1}{2}(n-1)$ hairpins, and pknot(*M*) is the crossing number of the deflated matching, which is the number of hairpins. Thus pknot_{max}(CC_n) = $\frac{1}{2}(n-1)$.

Example 4.4. Suppose we want to calculate the maximum pseudoknot numbers for the C&C families with four and five edges.

First, let n = 4. According to Theorem 4.4, $pknot_{max}(M) = 2$. Figure 24 shows the matching with this pseudoknot number.

Now, let n = 5. By Theorem 4.4, the maximum pseudoknot will be just like n = 4. With the extra edge, we can either insert it into the allowable space or inflate the original matching. If we conduct an insertion, we will not increase the crossing number, unlike inflating. However, this one edge will become deflated. Figure 25 shows matchings which produce a maximum pseudoknot number of 2 on n = 5 edges.



Figure 25. Matchings that give the maximum pseudoknot number on five edges for the C&C family.



Figure 26. Matching that gives the maximum pseudoknot number on five edges for all perfect matchings.

Theorem 4.5. *The maximum pseudoknot number of the set of all perfect matchings on n edges is given by*

$$pknot_{max}(M_n) = \frac{1}{2}n(n-1)$$

Proof. The only restrictions we have on all perfect matchings are that an edge cannot cross itself or go below the horizon. In order to maximize $pknot(M_n)$ in a perfect matching, none of the edges should be involved in ladders, and each edge should cross every edge in the matching once. The way to maximize $pknot(M_n)$ for any given n is to use the matching on n-1 edges with the maximum pseudoknot number, and cross all of those edges with the new edge we add. Thus, we can represent this as the recurrence relation $pknot_{max}(M_n) = pknot_{max}(M_{n-1}) + (n-1)$ with the initial condition $pknot_{max}(M_2) = 1$ and where (n-1) represents how many edges our new edge will cross. Solving this recurrence relation gives $\frac{1}{2}n(n-1)$.

Example 4.5. Suppose we want to find $pknot_{max}(M_n)$ for all perfect matchings on n = 5 edges.

According to Theorem 4.5, $pknot_{max}(M_5) = \frac{5(4)}{2} = 10$. Figure 26 shows the matching with the maximum pseudoknot number.

4F. *Comparison.* Pseudoknots are not found as commonly in RNA secondary structures as they are in perfect matchings. One desired result of the inductive definitions of L&P and C&C is that the models more accurately reflect the likelihood of pseudoknots observed in nature. The following graphs in Figures 27, 29, and 28 display the distributions of the crossing number, pseudoknot number, and nesting



278 N. ANDERSON, M. BREUNIG, K. GORYL, H. LEWIS, M. RIEHL AND M. SCANLAN

Figure 27. Percent of matchings on nine edges with given crossing number.



Figure 28. Percent of matchings on nine edges with given nesting number.

number for each given family on nine edges as a percentage of the total matchings in that family. The motivation for this section is to examine how limiting the number of pseudoknots affects the crossing, nesting, and pseudoknot number distribution compared to all perfect matchings.

In all perfect matchings the crossing and nesting number statistics are symmetrically distributed and their joint distribution has been an area of recent study.



Figure 29. Percent of matchings on nine edges with given pseudoknot number.

Note that in all perfect matchings on *n* edges, as the crossing number increases, the nesting number decreases, and vice versa. These two statistics are inversely related and symmetrically distributed when considering all perfect matchings [Chen et al. 2007]. However, when we limit the number of pseudoknots by looking at L&P and C&C matchings, the distributions for crossing number and pseudoknot number become skewed right. Because the crossing and nesting number statistics are inversely related when considering all perfect matchings we would predict that the nesting number distribution would become skewed left when considering these L&P and C&C matchings. Surprisingly, the distributions of nesting numbers for L&P and C&C remain largely similar to the distribution of nesting numbers for all matchings. However, recall that these matching families limit the unlikely biological structures, in this case a high number of pseudoknots. Pseudoknots are represented in matchings by a hairpin, ignoring the additional ladders. Therefore these matchings limit the number of hairpins, so we should expect there to be more matchings with a smaller crossing number. These matching families don't limit the ladders that can occur on edges or newly inserted edges in a hairpin, so the nesting number stays relatively symmetrically distributed.

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2019 vol. 12 no. 2

Lights Out for graphs related to one another by constructions	181
LAURA E. BALLARD, ERICA L. BUDGE AND DARIN R.	
Stephenson	
A characterization of the sets of periods within shifts of finite type	203
MADELINE DOERING AND RONNIE PAVLOV	
Numerical secondary terms in a Cohen–Lenstra conjecture on real	221
quadratic fields	
Codie Lewis and Cassandra Williams	
Curves of constant curvature and torsion in the 3-sphere	235
Debraj Chakrabarti, Rahul Sahay and Jared	
WILLIAMS	
Properties of RNA secondary structure matching models	257
NICOLE ANDERSON, MICHAEL BREUNIG, KYLE GORYL,	
HANNAH LEWIS, MANDA RIEHL AND MCKENZIE SCANLAN	
Infinite sums in totally ordered abelian groups	281
GREG OMAN, CAITLIN RANDALL AND LOGAN ROBINSON	
On the minimum of the mean-squared error in 2-means clustering	301
BERNHARD G. BODMANN AND CRAIG J. GEORGE	
Failure of strong approximation on an affine cone	321
Martin Bright and Ivo Kok	
Quantum metrics from traces on full matrix algebras	329
Konrad Aguilar and Samantha Brooker	
Solving Scramble Squares puzzles with repetitions	343
JASON CALLAHAN AND MARIA MOTA	
Erdős–Szekeres theorem for cyclic permutations	351
Éva Czabarka and Zhiyu Wang	

