RNA PSEUDOKNOT STRUCTURES WITH ARC-LENGTH \( \geq 3 \) AND STACK-LENGTH \( \geq \sigma \)

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\textbf{Abstract.} In this paper we enumerate \( k \)-noncrossing RNA pseudoknot structures with given minimum arc- and stack-length. That is, we study the numbers of RNA pseudoknot structures with arc-length \( \geq 3 \), stack-length \( \geq \sigma \) and in which there are at most \( k - 1 \) mutually crossing bonds, denoted by \( T_{k,\sigma}^{[3]}(n) \). In particular we prove that the numbers of 3, 4 and 5-noncrossing RNA structures with arc-length \( \geq 3 \) and stack-length \( \geq 2 \) satisfy

\[ T_{3,2}^{[3]}(n) \sim K_3 n^{2.5723n}, \quad T_{4,2}^{[3]}(n) \sim K_4 n^{-2.0306n}, \quad \text{and} \quad T_{5,2}^{[3]}(n) \sim K_5 n^{-1.4092n}, \]

respectively, where \( K_3, K_4, K_5 \) are constants. Our results are of importance for prediction algorithms for RNA pseudoknot structures.

\section{Introduction}

An RNA structure is the helical configuration of an RNA sequence, described by its primary sequence of nucleotides A, G, U and C together with the Watson-Crick (A-U, G-C) and (U-G) base pairing rules specifying which pairs of nucleotides can potentially form bonds. Subject to these single stranded RNA form helical structures. The function of many RNA sequences is often tantamount to their structures. Therefore it is of central importance to understand RNA structure in the context of studying the function of biological RNA, and in the design process of artificial RNA. In this paper we enumerate \( k \)-noncrossing RNA structures with arc-length \( \geq 3 \) and stack-length \( \geq \sigma \), where \( \sigma \geq 2 \). The main idea is to consider a certain subset of \( k \)-noncrossing core-structures, that is structures with minimum arc length 2, in which there exists no two arcs of the form \((i, j), (i+1, j-1)\) and no arcs of the form \((i, i+2)\) with isolated \( i+1 \). We prove a bijection between this subset of core structures with multiplicities and \( k \)-noncrossing RNA structures with arc-length \( \geq 3 \) and stack-length \( \geq \sigma \), where \( \sigma \geq 2 \). Subsequently, we derive several functional

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equations of generating functions, based on which transfer theorems imply our asymptotic formulas. The paper is relevant for prediction algorithms of pseudoknot RNA since it proves that the numbers of $k$-noncrossing RNA structures with arc-length $\geq 3$ and stack-length $\geq \sigma$ exhibit small exponential growth rates. The results suggest a novel strategy for RNA pseudoknot prediction.

2. Diagrams, matchings and structures

A diagram is labeled graph over the vertex set $[n] = \{1, \ldots, n\}$ with degree $\leq 1$, represented by drawing its vertices $1, \ldots, n$ in a horizontal line and its arcs $(i,j)$, where $i < j$, in the upper halfplane. The vertices and arcs correspond to nucleotides and Watson-Crick ($A-U$, $G-C$) and ($U-G$) base pairs, respectively.

![Figure 1. $k$-noncrossing diagrams. Top: 3-noncrossing diagram with arc-length $\geq 3$, (2,5), (7,10), the arc (7,10) being isolated. Hence we have a 3-noncrossing diagram $\lambda = 3$, $\sigma = 1$ diagram without isolated vertices. Bottom: 3-noncrossing (no red/purple cross), $\lambda = 4$, $\sigma = 2$ diagram with isolated vertices 13.](image)

We categorize diagrams according to the maximum number of mutually crossing arcs, $k - 1$, the minimum arc-length, $\lambda$, and the minimum stack-length, $\sigma$. Here the length of an arc $(i,j)$ is $j - i$ and a stack of length $\sigma$ is a sequence of “parallel” arcs of the form $((i,j), (i+1, j-1), \ldots, (i+(\sigma-1), j-(\sigma-1)))$. In the following we call a $k$-noncrossing diagram with arc-length $\geq 2$ and stack-length $\geq \sigma$ a $k$-noncrossing RNA structure. We denote the set (number) of $k$-noncrossing RNA
structures with stack-size $\geq \sigma$ by $T_{k,\sigma}(n)$ ($T_{k,\sigma}^{[3]}(n)$) and refer to $k$-noncrossing RNA structures for $k \geq 3$ as pseudoknot RNA structures. A $k$-noncrossing core-structure is a $k$-noncrossing RNA structures in which there exists no two arcs of the form $(i,j)$, $(i+1,j-1)$. We denote the set (number) of core-structures having $h$ arcs by $C_{k}(n,h)$ ($C_{k}(n,h)^{[3]}$) and $C_{k}(n)$ ($C_{k}(n)^{[3]}$) denotes the set (number) of core-structures. The set (number) of RNA structures with arc-length $\geq 3$, is denoted by $T_{k,\sigma}^{[3]}(n)$ ($T_{k,\sigma}^{[3]}(n)^{[3]}$). For $k = 2$ we have RNA structures with no crossing arcs, i.e. the well-known RNA secondary structures, whose combinatorics was pioneered by Waterman et al. $[18, 29, 30, 32, 31]$. RNA secondary structures are $T_{2,1}(n)$-structures. We denote by $f_{k}(n,\ell)$ the number of $k$-noncrossing diagrams with arbitrary arc-length and $\ell$ isolated points over $n$ vertices. In Figure 2 we display the various types of diagrams involved.

![Figure 2](image.png)

**Figure 2.** Basic diagram types: (a) perfect matching ($f_{3}(8,0)$), (b) partial matching with 1-arc $(5,6)$ and isolated points $2,7$ ($f_{3}(8,2)$), (c) structure with arc-length $\geq 3$ and stack-length $\geq 2$ and no isolated points ($T_{3,2}^{[3]}(8)$) and (d) structure with arc-length $\geq 3$, stack-length $\geq 3$ and isolated points $4,5$ ($T_{3,3}^{[3]}(8)$).

The following identities are due to Grabiner et al. $[9]

\begin{align}
\sum_{n \geq 0} f_{k}(n,0) \frac{x^{n}}{n!} &= \det[I_{i-j}(2x) - I_{i+j}(2x)]_{i,j=1}^{k-1} \\
\sum_{n \geq 0} \left\{ \sum_{\ell=0}^{n} f_{k}(n,\ell) \right\} \cdot \frac{x^{n}}{n!} &= e^{x} \det[I_{i-j}(2x) - I_{i+j}(2x)]_{i,j=1}^{k-1},
\end{align}

where $I_{r}(2x) = \sum_{j \geq 0} \frac{x^{2j+r}}{j!(r+j)!}$ denotes the hyperbolic Bessel function of the first kind of order $r$. Eq. (2.1) and (2.2) allow “in principle” for explicit computation of the numbers $f_{k}(n,\ell)$. In particular for $k = 2$ and $k = 3$ we have the formulas

\begin{align}
f_{2}(n,\ell) &= \binom{n}{\ell} C_{(n-\ell)/2} \quad \text{and} \quad f_{3}(n,\ell) = \binom{n}{\ell} \left[ C_{\frac{n-\ell}{2}}^{2} + 2C_{\frac{n-\ell}{2}} - C_{\frac{n-\ell+1}{2}}^{2} \right],
\end{align}
where \( C_m \) denotes the \( m \)-th Catalan number. \( f_3(n, \ell) \) results from a determinant formula enumerating pairs of nonintersecting Dyck-paths. In view of \( f_k(n, \ell) = \binom{n}{\ell} f_k(n - \ell, 0) \) everything can be reduced to perfect matchings, where we have the following situation: there exists an asymptotic approximation of the hyperbolic Bessel function due to [17] and employing the subtraction of singularities-principle [17] one can prove

\[
\forall k \in \mathbb{N}; \quad f_k(2n, 0) \sim \varphi_k(n) \left( \frac{1}{\rho_k} \right)^n,
\]

where \( \rho_k \) is the dominant real singularity of \( \sum_{n \geq 0} f_k(2n, 0) z^n \) and \( \varphi_k(n) \) is a polynomial over \( n \).

Via Hadamard’s formula, \( \rho_k \) can be expressed as

\[
\rho_k = \lim_{n \to \infty} \left( f_k(2n, 0) \right)^{-\frac{1}{n}}.
\]

Eq. (2.4) allows for any given \( k \geq 2 \) to obtain \( \varphi_k(n) \), explicitly.

As for the generating function and asymptotics of \( k \)-noncrossing RNA structures we have the following results from [10, 11, 12]. First the number of \( k \)-noncrossing RNA structures with \( (n - \ell/2) \) arcs, \( T_{k,1}(n, n-\ell/2) \), and the number of \( k \)-noncrossing RNA structures, \( T_{k,1}(n) \), are given by

\[
T_{k,1}(n, \frac{n - \ell}{2}) = \sum_{b=0}^{\lfloor n/2 \rfloor} (-1)^b \binom{n - b}{b} f_k(n - 2b, \ell)
\]

\[
T_{k,1}(n) = \sum_{b=0}^{\lfloor n/2 \rfloor} (-1)^b \binom{n - b}{b} \left\{ \sum_{\ell=0}^{n-2b} f_k(n - 2b, \ell) \right\},
\]

where \( \left\{ \sum_{\ell=0}^{n-2b} f_k(n - 2b, \ell) \right\} \) is given via eq. (2.2). Secondly we have

\[
T_{3,1}(n) \sim \frac{10.4724 \cdot 4!}{n(n-1) \ldots (n-4)} \left( \frac{5 + \sqrt{21}}{2} \right)^n
\]

\[
T_{[3],3,1}(n) \sim \frac{6.11170 \cdot 4!}{n(n-1) \ldots (n-4)} 4.54920^n.
\]

The particular class of \( k \)-noncrossing core-structures, i.e. structures in which there exists no two arcs of the form \((i,j), (i+1, j-1)\) will play a central role in the following enumerations:

**Theorem 1.** [13] (Core-structures) Suppose \( k \in \mathbb{N}, k \geq 2 \), let \( x \) be an indeterminant, \( \rho_k \) the dominant, positive real singularity of \( \sum_{n \geq 0} f_k(2n, 0) z^n \) (eq. (2.5)) and \( u_1(x) = \frac{1}{1+x^2} \). Then the
numbers of \( k \)-noncrossing core-structures over \([n]\), \( C_k(n) \) are given by

\[
C_k(n, h) = \sum_{b=0}^{h-1} (-1)^{h-b-1} \binom{h-1}{b} T_{k,1}(n-2h+2b+2, b+1).
\]

Furthermore we have the functional equation

\[
\sum_{n \geq 0} C_k(n) x^n = \frac{1}{u_1 x^2 - x + 1} \sum_{n \geq 0} f_k(2n, 0) \left( \frac{\sqrt{u_1 x}}{u_1 x^2 - x + 1} \right)^{2n}
\]

and

\[
C_k(n) \sim \frac{1}{\kappa_k} \left( \frac{1}{\rho_k} \right)^n
\]

where \( \kappa_k \) is a dominant singularity of \( \sum_{n \geq 0} C_k(n) \) and the minimal real solution of the equation \( \frac{\sqrt{u_1 x}}{u_1 x^2 - x + 1} = \rho_k \) and \( \varphi_k(n) \) is a polynomial over \( n \) derived from the asymptotic expression of \( f_k(2n, 0) \sim \varphi_k(n) \left( \frac{1}{\rho_k} \right)^n \) of eq. (2.4).

The following functional identity [11] relates the bivariate generating function for \( T_{k,1}(n, h) \), the number of RNA pseudoknot structures with \( h \) arcs to the generating function of \( k \)-noncrossing perfect matchings. It will be instrumental for the proof of Theorem 4 in Section 4.

**Lemma 1.** Let \( k \in \mathbb{N}, k \geq 2 \) and \( z, u \) be indeterminants over \( \mathbb{C} \). Then we have

\[
\sum_{n \geq 0} \sum_{h \leq n/2} T_{k,1}(n, h) u^{2h} z^n = \frac{1}{u^2 z^2 - z + 1} \sum_{n \geq 0} f_k(2n, 0) \left( \frac{u z}{u^2 z^2 - z + 1} \right)^{2n}.
\]

In particular we have for \( u = 1 \),

\[
\sum_{n \geq 0} T_{k,1}(n) z^n = \frac{1}{z^2 - z + 1} \sum_{n \geq 0} f_k(2n, 0) \left( \frac{z}{z^2 - z + 1} \right)^{2n}.
\]

In view of Lemma 1 it is of interest to deduce relations between the coefficients from the equality of generating functions. The class of theorems that deal with this deduction are called transfer-theorems [7]. One key ingredient in this framework is a specific domain in which the functions in question are analytic, which is “slightly” bigger than their respective radius of convergence. It is tailored for extracting the coefficients via Cauchy’s integral formula: given two numbers \( \phi, R \), where \( R > 1 \) and \( 0 < \phi < \frac{\pi}{2} \) and \( \rho \in \mathbb{R} \) the open domain \( \Delta_{\rho}(\phi, R) \) is defined as

\[
\Delta_{\rho}(\phi, R) = \{ z \mid |z| < R, z \neq \rho, |\text{Arg}(z - \rho)| > \phi \}
\]
A domain is a $\Delta_\rho$-domain if it is of the form $\Delta_\rho(\phi, R)$ for some $R$ and $\phi$. A function is $\Delta_\rho$-analytic if it is analytic in some $\Delta_\rho$-domain. We use the notation

\begin{equation}
(2.16) \quad (f(z) = O(g(z)) \text{ as } z \to \rho) \iff (f(z)/g(z) \text{ is bounded as } z \to \rho)
\end{equation}

and if we write $f(z) = O(g(z))$ it is implicitly assumed that $z$ tends to a (unique) singularity. $[z^n]f(z)$ denotes the coefficient of $z^n$ in the power series expansion of $f(z)$ around 0.

**Theorem 2.** Let $f(z), g(z)$ be a $\Delta_\rho$-analytic functions given by power series $f(z) = \sum_{n \geq 0} a_n z^n$ and $g(z) = \sum_{n \geq 0} b_n z^n$. Suppose $f(z) = O(g(z))$ for all $z \in \Delta_\rho$ and $b_n \sim \varphi(n)(\rho^{-1})^n$, where $\varphi(n)$ is a polynomial over $n$. Then

\begin{equation}
(2.17) \quad a_n = [z^n]f(z) \sim K [z^n]g(z) = K b_n \sim K \varphi(n)(\rho^{-1})^n
\end{equation}

for some constant $K$.

### 3. Exact Enumeration

Our first result, Theorem 3, enumerates $k$-noncrossing RNA structures with arc-length $\geq 3$ and stack-length $\geq \sigma$. The structure of the formula is the exact analogue of the Möbius inversion of eq. (2.10) [13], which relates the numbers of all structures and the numbers of core-structures:

$T_{k,\sigma}(n, h) = \sum_{b=\sigma}^{n-2b} \binom{b+(2-\sigma)(h-b)-1}{h-b-1} C_k(n-2b, h-b)$. While the latter cannot be used in order to enumerate $k$-noncrossing structures with arc-length $\geq 3$, see Figure 3, the set

**Figure 3.** Core-structures will in general have 2-arcs: the structure $\delta \in T_{3,2}(12)$ (lhs) is mapped into its core $c(\delta)$ (rhs). Clearly $\delta$ has arc-length $\geq 4$ and as a consequence of the collapse of the stack $((i+1, j+3), (i+2, j+2), (i+3, j))$ (the purple arcs are being removed) into the arc $(i+3, j)$, $c(\delta)$ contains the arc $(i, i+4)$, which is, after relabeling, a 2-arc.
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(3.1) $C^*_k(n, h) = \{\delta \mid \delta \in C_k(n, h); \exists (i, i + 2); i + 1 \text{ is an isolated vertex.} \}$

turns out to be the key.

**Theorem 3.** Suppose we have $k, h, \sigma \in \mathbb{N}, k \geq 2, h \leq n/2$ and $\sigma \geq 2$. Then the numbers of $k$-noncrossing RNA structures with arc-length $\geq 3$ and stack-length $\geq \sigma$ having $h$ arcs is given by

(3.2) $T^{[3]}_{k, \sigma}(n, h) = \sum_{b=\sigma-1}^{h-1} \binom{b + (2 - \sigma)(h - b) - 1}{h - b - 1} C^*_k(n - 2b, h - b)$

where $C^*_k(n, h)$ satisfies

(3.3) $C^*_k(n, h) = \sum_{j=0}^{h} (-1)^j \binom{n - 2j}{j} C_k(n - 3j, h - j)$

and $C_k(n', h')$ is given by Theorem 1.

| $n$ | 1  | 2  | 3  | 4  | 5  | 6  | 7  | 8  | 9  | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 |
|-----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
| $T^{[3]}_{k, \sigma}(n)$ | 1  | 1  | 1  | 1  | 2  | 4  | 9  | 19 | 40 | 82 | 167| 334| 682| 1398| 2917| 6142| 13025|
| $T^{[3]}_{k, h}(n)$      | 1  | 1  | 1  | 1  | 1  | 2  | 4  | 8  | 14 | 24 | 40 | 68 | 118| 209 | 371 | 654 |

**Proof.** We consider $C^*_k(n, h)$ (eq. 3.1) and call an arc $(i, i + 2)$ with isolated $i + 1$ a bad arc. It is straightforward to show that there are $\binom{n - 2j}{j}$ ways to select $j$ bad arcs over $[n]$. Since removing a bad arc by construction removes 3 vertices we observe that the number of configurations of at least $j$ bad arcs is given by $\binom{n - 2j}{j} C_k(n - 3j, h - j)$. Via the inclusion-exclusion principle we accordingly arrive at

(3.4) $C^*_k(n, h) = \sum_{j=0}^{h} (-1)^j \binom{n - 2j}{j} C_k(n - 3j, h - j)$.

We next observe that there exists a mapping from $k$-noncrossing structures with $h$ arcs with arc-length $\geq 3$ and stack-length $\sigma \geq 2$ over $[n]$ into $\bigcup_{\sigma - 1 \leq b \leq h - 1} C_k^*(n - 2b, h - b)$:

(3.5) $c: T^{[3]}_{k, \sigma}(n, h) \rightarrow \bigcup_{0 \leq b \leq h - 1} C_k^*(n - 2b, h - b), \quad \delta \mapsto c(\delta)$

which is obtained in two steps: first induce $c(\delta)$ by mapping arcs and isolated vertices as follows:

(3.6) $\forall \ell \geq \sigma - 1; \quad ((i - \ell, j + \ell), \ldots, (i, j)) \mapsto (i, j) \quad \text{and} \quad j \mapsto j$ if $j$ is an isolated vertex

and secondly relabel the resulting diagram from left to right in increasing order, see Figure 4.

**Claim 1.** $c: T^{[3]}_{k, \sigma}(n, h) \rightarrow \bigcup_{\sigma - 1 \leq b \leq h - 1} C_k^*(n - 2b, h - b)$ is well-defined and surjective.
By construction, \( c \) does not change the crossing number. Since \( T_{k,\sigma}^{[3]}(n) \) contains only arcs of length \( \geq 3 \) we derive \( c(T_{k,\sigma}^{[3]}(n)) \subset C_k^*(n-2b, h-b) \). Therefore \( c \) is well-defined. It remains to show that \( c \) is surjective. For this purpose let \( \delta \in C_k^*(n-2b, h-b) \) and set \( a = b - (\sigma - 1)(h-b) \). We proceed constructing a \( k \)-noncrossing structure \( \tilde{\delta} \) in three steps:

**Step 1.** replace each label \( i \) by \( r_i \), where \( r_i \leq r_s \) if and only if \( i \leq s \).

**Step 2.** replace the leftmost arc \((r_p, r_q)\) by the sequence of arcs

\[
((\tau_p - (\lfloor \sigma - 1 \rfloor + a), \tau_q + (\lfloor \sigma - 1 \rfloor + a)), \ldots, (\tau_p, \tau_q))
\]

and each isolated vertex \( r_s \) by \( \tau_s \).

**Step 3.** Set for \( x, y \in \mathbb{Z}, \tau_b + y \leq \tau_c + x \) if and only if \( b < c \) or \( b = c \) and \( y \leq x \). By construction, \( \leq \) is a linear order over

\[
n - 2b + 2(h - b)(\sigma - 1) + 2a = n - 2b + 2(h - b)(\sigma - 1) + 2(b - (\sigma - 1)(h-b)) = n
\]
elements, which we then label from 1 to \( n \) (left to right) in increasing order. It is straightforward to verify that \( c(\tilde{\delta}) = \delta \) holds. It remains to show that \( \tilde{\delta} \in T_{k,\sigma}^{[3]}(n) \). Suppose \textit{a contrario} \( \tilde{\delta} \) contains an arc \((i, i + 2)\). Since \( \sigma \geq 2 \) we can then conclude that \( i + 1 \) is necessarily isolated. The arc \((i, i + 2)\) is mapped by \( c \) into \((j, j + 2)\) with isolated point \( j + 1 \), which is impossible by definition of \( C_k^*(n', h') \) and Claim 1 follows.

Labeling the \( h \) arcs of \( \delta \in T_{k,\sigma}^{[3]}(n, h) \) from left to right and keeping track of multiplicities gives rise to the map

\[
f_{k,\sigma}^{[3]} : T_{k,\sigma}^{[3]}(n, h) \to \bigcup_{0 \leq b \leq h-1} C_k^*(n-2b, h-b) \times \left\{ (a_j)_{1 \leq j \leq h-b} \mid \sum_{j=1}^{h-b} a_j = b, \ a_j \geq \sigma - 1 \right\},
\]
given by $f_{k,\sigma}(\delta) = (c(\delta), (a_j)_{1 \leq j \leq h-b})$. We can conclude that $f_{k,\sigma}$ is well-defined and a bijection. We proceed computing the multiplicities of the resulting core-structures [13]:

$$|\{(a_j)_{1 \leq j \leq b} \mid \sum_{j=1}^{b-h} a_j = b; a_j \geq \sigma - 1\}| = \binom{b + (2 - \sigma)(h-b) - 1}{h-b-1}.$$  

Eq. (3.10) and eq. (3.9) imply

$$T_{k,\sigma}^{[3]}(n, h) = \sum_{b=0}^{h-1} \binom{h-b-1}{b=\sigma-1} \binom{b + (2 - \sigma)(h-b) - 1}{h-b-1} C_k^*(n - 2b, h-b),$$

and the theorem follows.  

We proceed by proving a functional identity between the bivariate generating functions of $T_{k,\sigma}^{[3]}(n, h)$ and $C_k^*(n, h)$. This identity is based on Theorem 3 and crucial for proving Theorem 4 in Section 4. Its proof is analogous to Lemma 3 in [13].

**Lemma 2.** Let $k, \sigma \in \mathbb{N}$, $k \geq 2$ and let $u, x$ be indeterminants. Suppose we have

$$\forall h \geq 1; \quad A_{k,\sigma}(n, h) = \sum_{b=0}^{h-1} \binom{h-b-1}{b=\sigma-1} \binom{b + (2 - \sigma)(h-b) - 1}{h-b-1} B_k(n - 2b, h-b) \quad \text{and} \quad A_{k,\sigma}(n, 0) = 1.$$  

Then we have the functional relation

$$\sum_{n \geq 0} \sum_{h \leq \frac{n}{2}} A_{k,\sigma}(n, h) u^h x^n = \sum_{n \geq 0} \sum_{h \leq \frac{n}{2}} B_k(n, h) \left( \frac{u \cdot (ux)^{\sigma-1}}{1 - ux} \right)^{\frac{n}{h}} x^n + \frac{x}{1-x}.$$  

**Proof.** We set $\sum_{n \geq 0} \sum_{h \leq \frac{n}{2}} B_k(n, h) u^h x^n = \sum_{h \geq 0} \varphi_h(x) u^h$ and compute in view of eq. (3.12)

$$\sum_{n \geq 0} \sum_{h \leq \frac{n}{2}} A_{k,\sigma}(n, h) u^h x^n = \sum_{n \geq 0} \sum_{h \leq \frac{n}{2}} \sum_{b \leq h-1} B_k(n - 2b, h-b) \left( \frac{b + (2 - \sigma)(h-b) - 1}{h-b-1} \right) u^h x^n + \sum_{i \geq 1} x^i$$

where the term $\sum_{i \geq 1} x^i = \frac{x}{1-x}$ comes from the fact that for $h = 0$ the binomial

$$\binom{b + (2 - \sigma)(h-b) - 1}{h-b-1}$$
is zero, while for any $i \geq 1$ the lhs counts $A_{k,\sigma}(n, 0) = 1$. We proceed by computing

$$= \sum_{h \geq 0} \sum_{b \leq h} B_k(n - 2b, h - b) x^{n - 2b} \left( b + \frac{(2 - \sigma)(h - b) - 1}{h - b - 1} \right) u^b x^{2b} + \frac{x}{1 - x}$$

$$= \sum_{b \geq 0} \sum_{h \leq b} \varphi_{h - b}(x) \left( b + \frac{(2 - \sigma)(h - b) - 1}{h - b - 1} \right) u^b x^{2b} + \frac{x}{1 - x}.$$  

Setting $m = h - b$ and subsequently interchanging the summation indices we arrive at

$$\sum_{n \geq 0} \sum_{h \leq n} A_{k,\sigma}(n, h) u^b x^n = \sum_{m \geq 0} \sum_{b \leq m} \varphi_{m}(x) \left( b + \frac{(2 - \sigma)m - 1}{m - 1} \right) u^m \left( \frac{u \cdot (ux^2)^{\sigma - 1}}{1 - ux^2} \right)^{m - 1} + \frac{x}{1 - x}$$

$$= \sum_{m \geq 0} \varphi_{m}(x) \left( \frac{u \cdot (ux^2)^{\sigma - 1}}{1 - ux^2} \right)^{m - 1} + \frac{x}{1 - x}$$

$$= \sum_{n \geq 0} \sum_{h \leq n} B_k(n, h) \left( \frac{u \cdot (ux^2)^{\sigma - 1}}{1 - ux^2} \right)^{h - 1} + \frac{x}{1 - x},$$

whence Lemma 2. 

According to Lemma 2 and eq. (3.2) we have

$$T_{k,\sigma}(n, h) = \sum_{b = \sigma - 1}^{h - 1} \left( b + \frac{(2 - \sigma)(h - b) - 1}{h - b - 1} \right) C_k(n - 2b, h - b)$$

$$T_{k,\sigma}^{[3]}(n, h) = \sum_{b = \sigma - 1}^{h - 1} \left( b + \frac{(2 - \sigma)(h - b) - 1}{h - b - 1} \right) C_k^{*}(n - 2b, h - b).$$

and Lemma 2 implies the following two functional identities, which are instrumental for the proof of Theorem 4 in Section 4.

$$\sum_{n \geq 0} \sum_{h \leq n} T_{k,\sigma}(n, h) u^h x^n = \sum_{n \geq 0} \sum_{h \leq n} C_k(n, h) \left( \frac{u \cdot (ux^2)^{\sigma - 1}}{1 - ux^2} \right)^{h - 1} x^n + \frac{x}{1 - x}$$

$$\sum_{n \geq 0} T_{k,\sigma}^{[3]}(n) x^n = \sum_{n \geq 0} \sum_{h \leq n} C_k^{*}(n, h) \left( \frac{(ux^2)^{\sigma - 1}}{1 - x^2} \right)^{h} x^n + \frac{x}{1 - x}.$$
4. Asymptotic Enumeration

In this Section we study the asymptotics of \(k\)-noncrossing RNA pseudoknot structures with arc-length \(\geq 3\) and minimum stack length \(\sigma\). We are particularly interested in deriving simple formulas, that can be used assessing the complexity of prediction algorithms for \(k\)-noncrossing RNA structures. In order to state Theorem 4 below we introduce the following rational functions

\[
(4.1) \quad w_0(x) = \frac{x^{2\sigma-2}}{1-x^2} \\
(4.2) \quad z_0(x) = \frac{x}{1 + w_0(x)x^3} \\
(4.3) \quad u_0(x) = \frac{w_0}{1 + w_0(x)z_0(x)^2} \\
(4.4) \quad v_0(x) = \frac{1}{x u_0(x)z_0(x)^2 - z_0(x) + 1}.
\]

**Theorem 4.** Let \(k, \sigma \in \mathbb{N}, k, \sigma \geq 2, x\) be an indeterminant and \(\rho_k\) the dominant, positive real singularity of \(\sum_{n \geq 0} f_k(2n, 0)z^n\) (eq. (2.4)). Then \(T_{k,\sigma}^{[3]}(n)\), the number of RNA structures with arc-length \(\geq 3\) and \(\sigma \geq 2\) satisfies the following identity

\[
(4.5) \quad \sum_{n \geq 0} T_{k,\sigma}^{[3]}(n)z^n = v_0(0) \sum_{n \geq 0} f_k(2n, 0) \left( \frac{\sqrt{u_0(x)z_0(x)}}{u_0(x)z_0(x)^2 - z_0(x) + 1} \right)^{2n} + \frac{x}{1-x} - \frac{z_0(x)^2}{1-z_0(x)}
\]

where \(w_0(x), z_0(x), u_0(x), v_0(x)\) are given by eq. (4.1)–eq. (4.4). Furthermore

\[
(4.6) \quad T_{k,\sigma}^{[3]}(n) \sim \varphi_k(n) \left( \frac{1}{\gamma_{k,\sigma}} \right)^n
\]

holds, where \(\gamma_{k,\sigma}\) is the positive real dominant singularity of \(\sum_{n \geq 0} T_{k,\sigma}(n)z^n\) and minimal real solution of the equation

\[
(4.7) \quad \frac{\sqrt{u_0(x)z_0(x)}}{u_0(x)z_0(x)^2 - z_0(x) + 1} = \rho_k
\]

and \(\varphi_k(n)\) is a polynomial over \(n\) derived from the asymptotic expression of \(f_k(2n, 0) \sim \varphi_k(n) \left( \frac{1}{\rho_k} \right)^n\) of eq. (2.4).
Theorem 4 implies the following growth rates for 3-, 4- and 5-noncrossing RNA structures with arc-length \( \geq 3 \) and stack-length \( \geq 2, 3 \):

\[
\begin{align*}
(\gamma_{3,2})^{-1} &= 2.5723 & (\gamma_{4,2})^{-1} &= 3.0306 & (\gamma_{5,2})^{-1} &= 3.4092 \\
(\gamma_{3,3})^{-1} &= 2.0392 & (\gamma_{4,3})^{-1} &= 2.2663 & (\gamma_{5,3})^{-1} &= 2.4442 \\
\end{align*}
\]

Furthermore we compare in the following table the exact subexponential factors \( T_{k,3}^{[3]}(n) (\gamma_{k,2}^{[3]})^n \)
computed via Theorem 3 with the subexponential factors \( \varphi_k(n) \) obtained from Theorem 2.

| \( n \)   | \( T_{3,3}^{[3]}(n) (\gamma_{3,3}^{[3]})^n \) | \( T_{4,3}^{[3]}(n) (\gamma_{4,3}^{[3]})^n \) | \( T_{5,3}^{[3]}(n) (\gamma_{5,3}^{[3]})^n \) |
|----------|---------------------------------|---------------------------------|---------------------------------|
| 50       | \( 4.93 \times 10^{-5} \)     | \( 3.97 \times 10^{-6} \)     | \( 1.53 \times 10^{-10} \)     |
| 60       | \( 2.36 \times 10^{-5} \)     | \( 1.54 \times 10^{-6} \)     | \( 2.11 \times 10^{-11} \)     |
| 70       | \( 1.25 \times 10^{-5} \)     | \( 6.94 \times 10^{-7} \)     | \( 6.22 \times 10^{-12} \)     |
| 80       | \( 7.07 \times 10^{-6} \)     | \( 3.49 \times 10^{-7} \)     | \( 1.53 \times 10^{-12} \)     |
| 90       | \( 4.25 \times 10^{-6} \)     | \( 1.91 \times 10^{-7} \)     | \( 4.44 \times 10^{-13} \)     |
| 100      | \( 2.68 \times 10^{-6} \)     | \( 1.12 \times 10^{-7} \)     | \( 1.99 \times 10^{-13} \)     |

Proof. In the following we will use the notation \( w_0, u_0, z_0, \) eq. 4.1–eq. 4.4, for short without specifying the variable \( x \). The first step consists in deriving a functional equation relating the bivariate generating functions of \( C_k^{*}(n, h) \) and \( C_k(n', h') \). For this purpose we use eq. 3.3

\( C_k(n, h) = \sum_{b \leq \frac{h}{2}} (-1)^b \binom{n - 2b}{b} C_k(n - 3b, h - b) \).

Claim 1.

\[
(4.8) \quad \sum_{n \geq 0} \sum_{h \leq \frac{n}{2}} C_k(n, h) w^h x^n = \frac{1}{1 + wx} \sum_{n \geq 0} \sum_{h \leq \frac{n}{2}} C_k(n, h) w^h \left( \frac{x}{1 + wx} \right)^n.
\]

To prove Claim 1 we compute

\[
\sum_{n \geq 0} \sum_{h \leq \frac{n}{2}} C_k(n, h) w^h x^n = \sum_{n \geq 0} \sum_{h \leq \frac{n}{2}} \sum_{b \leq h} (-1)^b \binom{n - 2b}{b} C_k(n - 3b, h - b) w^h x^n = \sum_{n \geq 0} \sum_{h \leq \frac{n}{2}} \sum_{b \leq \frac{h}{2}} (-1)^b \binom{n - 2b}{b} C_k(n - 3b, h - b) w^h x^n.
\]
We rearrange the summation over \( h \) and arrive at

\[
\sum_{n \geq 0} \sum_{b \leq \frac{n}{2}} (-1)^b \binom{n-2b}{b} \left[ \sum_{h \leq \frac{n}{2}} C_k(n-3b, h-b) w^{h-b} \right] w^b x^n.
\]

Setting \( \varphi_n(w) = \sum_{j \leq \frac{n}{2}} C_k(n, j) w^j \) this becomes

\[
= \sum_{n \geq 0} \sum_{b \leq \frac{n}{2}} (-1)^b \binom{n-2b}{b} \varphi_{n-3b}(w) w^b x^n
\]

\[
= \sum_{b \geq 0} \frac{(-wx^3)^b}{b!} \sum_{n \geq 3b} \frac{(n-2b)!}{(n-3b)!} \varphi_{n-3b}(w) x^{n-3b} \quad \text{where} \quad m = n - 3b
\]

\[
= \sum_{m \geq 0} \frac{(m+b)!}{m!} \varphi_m(w) x^m
\]

\[
= \sum_{m \geq 0} \varphi_m(x) \frac{x^m}{m!} \sum_{b \geq 0} \frac{(-wx^3)^b}{b!} (m+b)!
\]

Laplace transformation of the series \( \sum_{b \geq 0} \frac{(m+b)!}{b!} y^b \) yields

\[
\sum_{b \geq 0} \frac{(m+b)!}{b!} y^b = \int_0^\infty \sum_{b \geq 0} \frac{y^b}{b!} t^{m+b} e^{-t} dt
\]

\[
= \int_0^\infty t^m e^{-(1-y)t} dt
\]

\[
= \frac{1}{(1-y)^{m+1}} \int_0^\infty ((1-y)t)^m e^{-(1-y)t} d((1-y)t)
\]

\[
= \frac{1}{(1-y)^{m+1}}.
\]

Hence the bivariate generating function can be written as

\[
\sum_{n \geq 0} \sum_{h \leq \frac{n}{2}} C^*_k(n, h) w^h x^n = \sum_{m \geq 0} \frac{\varphi_m(x)}{m!} \frac{m!}{(1+wx^3)^{m+1}}
\]

\[
= \frac{1}{1+wx^3} \sum_{m \geq 0} \varphi_m(w) \left( \frac{x}{1+wx^3} \right)^m
\]

\[
= \frac{1}{1+wx^3} \sum_{n \geq 0} \sum_{h \leq \frac{n}{2}} C_k(n, h) w^h \left( \frac{x}{1+wx^3} \right)^n
\]
and the Claim 1 follows. According to eq. (3.18), we have

\[
\sum_{n \geq 0} \sum_{h \leq n/2} C^*_k(n, h) \left( \frac{(x^2)^{\sigma-1}}{1-x^2} \right)^h x^n = \sum_{n \geq 0} \sum_{h \leq n/2} C^*_k(n, h) \left( \frac{1}{1-x^2} \right)^h x^n + \frac{x}{1-x},
\]

and Claim 1 provides, setting

\[
w_0 = \frac{(x^2)^{\sigma-1}}{1-x^2},
\]

the following interpretation of the rhs of eq. (4.9):

\[
\sum_{n \geq 0} \sum_{h \leq n/2} C^*_k(n, h) \left( \frac{(x^2)^{\sigma-1}}{1-x^2} \right)^h x^n = \frac{1}{1 + w_0x^3} \left[ \sum_{n \geq 0} \sum_{h \leq n/2} C_k(n, h)w_0^h \left( \frac{x}{1 + w_0x^3} \right)^n \right].
\]

According to eq. (3.17) and Lemma 1 we have

\[
\sum_{n \geq 0} \sum_{h \leq n/2} T_{k,1}(n, h)u^hz^n = \left[ \sum_{n \geq 0} \sum_{h \leq n/2} C_k(n, h) \left( \frac{u}{1-uz^2} \right)^h z^n \right] + \frac{z}{1-z}
\]

\[
\sum_{n \geq 0} \sum_{h \leq n/2} T_{k,1}(n, h)u^hz^n = \frac{1}{uz^2 - u + 1} \sum_{n \geq 0} f_k(2n, 0) \left( \frac{\sqrt{uz}}{uz^2 - z + 1} \right)^{2n}
\]

and consequently

\[
\sum_{n \geq 0} \sum_{h \leq n/2} C_k(n, h) \left( \frac{u}{1-uz^2} \right)^h z^n = \frac{1}{uz^2 - z + 1} \sum_{n \geq 0} f_k(2n, 0) \left( \frac{\sqrt{uz}}{uz^2 - z + 1} \right)^{2n} - \frac{z}{1-z}
\]

holds. Suppose now

\[
z_0(x) = \frac{x}{1 + w_0x^3} \]

\[
u_0(x) = \frac{w_0}{1 + w_0z_0^3}.
\]

Then we have the formal identity \( \frac{w_0}{1 - w_0z_0} = w_0 \) and obtain substituting eq. (4.11) into eq. (4.9)

\[
\sum_{n \geq 0} T_{k,2}^{[3]}(n)x^n = \frac{1}{1 + w_0x^3} \left[ \sum_{n \geq 0} \sum_{h \leq n/2} C_k(n, h)w_0^h \left( \frac{x}{1 + w_0x^3} \right)^n \right] + \frac{x}{1-x}
\]

Next we use eq. (4.12) and the formal identity \( \frac{w_0}{1 - w_0z_0} = w_0 \) to arrive at:

\[
\sum_{n \geq 0} T_{k,2}^{[3]}(n)x^n = \frac{1}{1 + w_0x^3} \left[ \sum_{n \geq 0} \sum_{h \leq n/2} C_k(n, h) \left( \frac{w_0}{1 - w_0z_0} \right)^h \right] + \frac{x}{1-x}.
\]
Setting $t_0(x) = \frac{1}{1+u_0x}$, $t_1(x) = \frac{x}{1-x}$ and $t_2(x) = \frac{z_0}{1-z_0}$ we derive via eq. (4.14)

\begin{equation}
\sum_{n \geq 0} T_{k,2}^{[3]}(n)x^n = t_0(x) \left[ \frac{1}{u_0z_0^2 - z_0 + 1} \sum_{n \geq 0} f_k(2n, 0) \left( \frac{\sqrt{u_0z_0^2}}{u_0z_0^2 - z_0 + 1} \right)^{2n} \right] - t_0(x)t_2(x) + t_1(x).
\end{equation}

We compute

\begin{align*}
t_0(x) &= \frac{x - x^3}{x^{2\sigma+1} - x^2 + 1} \\
t_1(x) - t_0t_2(x) &= \frac{f(x)}{(1 - x - x^2 + x^3 + x^{2\sigma+1})(x-1)(x^2 - 1 - x^{2\sigma+1})},
\end{align*}

where $f(x)$ is a polynomial of degree $4\sigma + 2$. Therefore $t_0(x)$ and $t_1(x) - t_0t_2(x)$ are analytic in $\{ z \in \mathbb{C} \mid 0 < |z| < \frac{1}{2} \}$ and accordingly do not introduce any singularities of

\begin{equation}
\frac{1}{u_0z_0^2 - z_0 + 1} \sum_{n \geq 0} f_k(2n, 0) \left( \frac{\sqrt{u_0z_0^2}}{u_0z_0^2 - z_0 + 1} \right)^{2n}
\end{equation}

in the domain $\{ z \in \mathbb{C} \mid 0 < |z| < \frac{1}{2} \}$. Furthermore we can conclude from eq. (4.17) that $x = 0$ is a removable singularity. Let us denote $V(z) = \sum_{n \geq 0} f_k(2n, 0) \left( \frac{\sqrt{u_0z_0^2}}{u_0z_0^2 - z_0 + 1} \right)^{2n}$.

**Claim 2.** All dominant singularities of $\sum_{n \geq 0} T_{k,2}^{[3]}(n)z^n$ are singularities of $V(z)$. Furthermore the unique, minimal, positive, real solution of

\begin{equation}
\frac{\sqrt{u_0z_0^2}}{u_0z_0^2 - z_0 + 1} = \rho_k
\end{equation}

denoted by $\gamma_{k,\sigma}^{[3]}$ is a dominant singularity of $\sum_{n \geq 0} T_{k,\sigma}^{[3]}(n)z^n$.

Clearly, a dominant singularity of $\frac{1}{u_0z_0^2 - z_0 + 1}V(z)$ is either a singularity of $V(z)$ or $\frac{1}{u_0z_0^2 - z_0 + 1}$. Suppose there exists some singularity $\zeta \in \mathbb{C}$ which is a root of $\frac{1}{u_0z_0^2 - z_0 + 1}$. By construction $\zeta \neq 0$ and $\zeta$ is necessarily a non-finite singularity of $V(z)$. If $|\zeta| \leq \gamma_{k,\sigma}^{[3]}$, then we arrive at the contradiction $|V(\zeta)| > |V(\rho_k)|$ since $V(\zeta)$ is not finite and

\begin{equation}
V(\rho_k) = \sum_{n \geq 0} f_k(2n, 0)\rho_k^{2n} < \infty.
\end{equation}

Therefore all dominant singularities of $\sum_{n \geq 0} T_{k,\sigma}^{[3]}(n)z^n$ are singularities of $V(z)$. According to Pringsheim’s Theorem [26], $\sum_{n \geq 0} T_{k,\sigma}^{[3]}(n)z^n$ has a dominant positive real singularity which by construction equals $\gamma_{k,\sigma}^{[3]}$ being the minimal positive real solution of

\begin{equation}
\frac{\sqrt{(x^2)^{\sigma-1}x}}{(x^2)^{\sigma-1}} x^2 - x + 1 = \rho_k
\end{equation}
and the Claim 2 follows.
Claim 2 immediately implies that the inverse of $\gamma_{k,\sigma}^{[3]}$ equals the exponential growth-rate. According to $\gamma_{k,\sigma}^{[2]}$ the power series $\sum_{n \geq 0} f_k(2n,0)z^n$ has an analytic continuation in a $\Delta_{\rho_k}$-domain and we have $[z^n]V(z) \sim K\varphi_k(n)(\rho^{-1})^n$, where $\varphi_k(n)$ is given by eq. (2.4). We can therefore employ Theorem $\gamma_{k,\sigma}^{[2]}$ which allows us to transfer the subexponential factors from the asymptotic expressions for $f_k(2n,0)$ to $T_{k,\sigma}(n)$ and eq. (4.6) follows. This completes the proof of Theorem $\gamma_{k,\sigma}^{[3]}$. □

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