Combinatorics of $\gamma$-structures

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Received: date / Accepted: date

Abstract In this paper we study canonical $\gamma$-structures, a class of RNA pseudoknot structures that plays a key role in the context of polynomial time folding of RNA pseudoknot structures. A $\gamma$-structure is composed of specific building blocks, that have topological genus less than or equal to $\gamma$, where composition means concatenation and nesting of such blocks. Our main result is the derivation of the generating function of $\gamma$-structures via symbolic enumeration. $\gamma$-structures are constructed via $\gamma$-matchings. We compute an algebraic equation for the generating function of these matchings and prove that it is the unique solution. For $\gamma = 1$ and $\gamma = 2$ we compute the Puiseux-expansion of this power series at its unique, dominant singularity. This allows us to derive simple asymptotic formulas for the number of 1-structures and 2-structures.

Keywords generating function · shape · irreducible shadow · $\gamma$-structure

1 Introduction and background

An RNA sequence is a linear, oriented sequence of the nucleotides (bases) A,U,G,C. These sequences “fold” by establishing bonds between pairs of nucleotides. These bonds cannot form arbitrarily, a nucleotide can at most establish one bond and the global conformation of an RNA molecule is determined by topological constraints encoded at the level of secondary structure, i.e., by the mutual arrangements of the base pairs [Baior et al. (2010)]. Secondary structures can be interpreted as (partial) matchings in a graph of permissible base pairs [Tabaska et al. (1998a)]. When represented as a diagram, i.e. as a graph whose vertices are drawn on a horizontal line with arcs in the upper halfplane on refers to a secondary structure with crossing arcs as a pseudoknot structure.

Folded configurations are energetically optimal. Here energy means free energy, which is dominated by the stacking of adjacent base pairs and not by the hydrogen
bonds of the individual base pairs [Mathews et al. 1999], as well as minimum arc-length conditions [Smith and Waterman 1978]. That is, a stack is tantamount to a sequence of parallel arcs \( ((i, j), (i + 1, j - 1), \ldots, (i + \tau, j - \tau)) \). In particular, only configurations without isolated bonds and without bonds of length one (formed by immediately subsequent nucleotides) are observed in RNA structures. For a given RNA sequence polynomial-time dynamic programming (DP) algorithms can be devised, finding such minimal energy configurations.

The topological classification of RNA structures [Bon et al. 2008; Andersen et al. 2011a] has recently been translated into an efficient dynamic programming algorithm [Reidys et al. 2011]. This algorithm a priori folds into a novel class of pseudoknot structures, the \( \gamma \)-structures. \( \gamma \)-structures differ from pseudoknotted RNA structures of fixed topological genus of an associated fatgraph or double line graph [Orland and Zee 2002] and [Bon et al. 2008], since they have arbitrarily high genus. They are composed by irreducible subdiagrams whose individual genus is bounded by \( \gamma \) and contain no bonds of length one (1-arcs), see Section 2 for details. The folding of \( \gamma \)-structures has led to unprecedented sensitivity and positive predictive value [Reidys et al. 2011].

In [Nebel and Weinberg 2011a] Nebel and Weinberg study a plethora of RNA structures appearing in the context of DP folding routines by means of multiple context-free grammars. From these grammars algebraic equations are devised for the generating functions of the corresponding structure classes. The authors study the case \( \gamma = 1 \) and find that in the limit of large \( n \) there are \( j_{1/1} n^{-3/2} (\varphi_{1/1}^{-1})^n \), 1-structures, where \( \varphi_{1/1}^{-1} = 3.8782 \) and \( j_1 \) is some positive constant. The presentation in [Nebel and Weinberg 2011a] however has its main focus on other aspects of pseudoknots (like e.g. a framework for their classification and comparison). Accordingly, the authors only sketch the way asymptotics for the number of different structures has been computed, neither discussing irreducibility of polynomial equations nor uniqueness of power series solutions.

In this paper we study canonical \( \gamma \)-structures, i.e. partial matchings composed by irreducible motifs of genus \( \leq \gamma \), without isolated arcs and 1-arcs. Due to the extended stacking of arcs canonical \( \gamma \)-structures are realistic folding targets of minimum free energy DP-algorithms. We identify a polynomial \( P_1(u, X) \), whose unique solution equals the generating function of \( \gamma \)-matchings. We then have a closer look at the cases \( \gamma = 1, 2 \) and prove that \( P_1(u, X) \) and \( P_2(u, X) \) are irreducible. This fact is of importance for interpreting the generating function of \( \gamma \)-matchings at its unique dominant singularity as a Puiseux-series, which in turn implies, by means of transfer theorems [Flajolet and Sedgewick 2009], simple asymptotic formulas for the numbers of \( \gamma \)-matchings.

\( \gamma \)-matchings are the stepping stone to derive via Lemma 4 the further refined, bivariate generating function of \( \gamma \)-shapes, i.e. \( \gamma \)-matchings containing only stacks composed by a single arc. This generating function keeps additionally track of the 1-arcs, that are vital for the later inflation into \( \gamma \)-structures. We then compute the generating function of \( \tau \)-canonical \( \gamma \)-structures inflating \( \gamma \)-shapes by means of symbolic enumeration. In the process we rediscover and generalize Nebel and Weinberg’s formula to arbitrary \( \gamma \).
2 Some basic facts

2.1 \( \gamma \)-diagrams

A diagram is a labeled graph over the vertex set \( [n] = \{1, \ldots, n\} \) in which each vertex has degree \( \leq 3 \), represented by drawing its vertices in a horizontal line. The backbone of a diagram is the sequence of consecutive integers \( (1, \ldots, n) \) together with the edges \( \{(i, i+1) \mid 1 \leq i \leq n-1\} \). The arcs of a diagram, \((i, j)\), where \( i < j \), are drawn in the upper half-plane. We shall distinguish the backbone edge \((i, i+1)\) from the arc \((i, i+1)\), which we refer to as a 1-arc.

A stack of length \( \tau \) is a maximal sequence of “parallel” arcs,

\[ ((i, j), (i+1, j-1), \ldots, (i+\tau, j-\tau)). \]

A stack of length \( \geq \tau \) is called a \( \tau \)-canonical stack, i.e. a stack of length zero is an isolated arc. The particular arc \((1, n)\) is called a rainbow and an arc is called maximal if it is maximal with respect to the partial order \((i, j) \leq (i', j')\) iff \( i' \leq i \land j \leq j' \), see Fig. 1.

A stack of length \( \tau \), \(((i, j), (i+1, j-1), \ldots, (i+\tau, j-\tau))\) induces a sequence of pairs \(((i, i+1), [j, j-1]), ([i+1, i+2], [j-1, j-2]) \ldots\). We call any of these \( 2\tau \) intervals a \( P \)-interval. The interval \([i+\tau, j-\tau]) \) is called a \( \sigma \)-interval, see Fig. 2.
We shall consider diagrams as fatgraphs, $G$, that is graphs $G$ together with a collection of cyclic orderings, called fattenings, one such ordering on the half-edges incident on each vertex. Each fatgraph $G$ determines an oriented surface $F(G)$ [Loebl and Moffatt (2008); Penner et al. (2010)] which is connected if $G$ is and has some associated genus $g(G) \geq 0$ and number $r(G) \geq 1$ of boundary components. Clearly, $F(G)$ contains $G$ as a deformation retract [Massey (1967)]. Fatgraphs were first applied to RNA secondary structures in Penner and Waterman (1993a) and Penner (2004).

A diagram $G$ hence determines a unique surface $F(G)$ (with boundary). Filling the boundary components with discs we can pass from $F(G)$ to a surface without boundary. Euler characteristic, $\chi$, and genus, $g$, of this surface is given by $\chi = v - e + r$ and $g = 1 - \frac{1}{2} \chi$, respectively, where $v, e, r$ is the number of discs, ribbons and boundary components in $G$, [Massey (1967)]. The genus of a diagram is that of its associated surface without boundary.

The shadow of a diagram of genus $g$ is obtained by removing all noncrossing arcs, deleting all isolated vertices and collapsing all induced stacks (i.e., maximal subsets of subsequent, parallel arcs) to single arcs, see Fig. 3.

A diagram $G$ can possibly be empty. Furthermore, projecting into the shadow does not affect genus. Any shadow of genus $g$ over one backbone contains at least $2g$ and at most $(6g - 2)$ arcs. In particular, for fixed genus $g$, there exist only finitely many shadows [Reidys et al. (2011); Andersen et al. (2011)]. In Fig. 4 we display the four shadows of genus one.

We denote shadows by $\sigma$.

A diagram is called irreducible, if and only if for any two arcs, $\alpha_1, \alpha_k$ contained in $E$, there exists a sequence of arcs $(\alpha_1, \alpha_2, \ldots, \alpha_{k-1}, \alpha_k)$ such that $(\alpha_1, \alpha_{i+1})$ are crossing. Irreducibility is equivalent to the concept of primitivity introduced by Bon et al. (2008), inspired by the work of Dyson (1949). According to Andersen et al. (2011), for arbitrary genus $g$ and $2g \leq \ell \leq (6g - 2)$, there exists an irreducible shadow of genus.
Fig. 5 A diagram $G$ is decomposed: we remove any noncrossing arcs and isolated points, collapse any stacks into a single arc and finally remove irreducible $G$-shadows from bottom to top and collapsing any stack generated in the process into a single arc.

Let $g$ having exactly $\ell$ arcs. We may reuse Fig. 4 as an illustration of this result since the four shadows of genus one are all irreducible.

Let $I_g(m)$ denote the number of irreducible shadows of genus $g$ with $m$ arcs. Since for fixed genus $g$ there exist only finitely many shadows we have the generating polynomial of irreducible shadows of genus $g$

$$I_g(z) = \sum_{m=2g}^{6g-2} i_g(m) z^m.$$

For instance for genus 1 and 2 we have

$$I_1(z) = z^2 + 2z^3 + z^4,$$

$$I_2(z) = 17z^4 + 160z^5 + 566z^6 + 1004z^7 + 961z^8 + 476z^9 + 96z^{10}.$$

The shadow $\sigma(G)$ of a diagram $G$ decomposes into a set of irreducible shadows. We shall call these shadows irreducible $G$-shadows.

Any diagram $G$ can iteratively be decomposed by first removing all noncrossing arcs as well as isolated vertices, second collapsing any stacks and third by removing irreducible $G$-shadows iteratively as follows, see Fig. 5:

- one removes (i.e. cuts the backbone at two points and after removal merges the cut-points) irreducible $G$-shadows from bottom to top, i.e. such that there exists no irreducible $G$-shadow that is nested within the one previously removed.
- if the removal of an irreducible $G$-shadow induces the formation of a stack, it is collapsed into a single arc.

A diagram, $\Gamma$, is a $\gamma$-diagram if and only if for any irreducible $G$-shadow, $G'$, $g(G') \leq \gamma$ holds.

We denote the set of $\tau$-canonical $\gamma$-diagrams by $\bar{G}_{\tau,\gamma}$. Such a diagram without arcs of the form $(i, i + 1)$ (1-arcs) is called a $\tau$-canonical $\gamma$-structure and their set is denoted by $\bar{G}_{\tau,\gamma}$. The set of $\gamma$-diagrams that contain only vertices of degree three ($\gamma$-matchings) is denoted by $\mathcal{G}_\gamma$ and the set of $\gamma$-matchings that contain only stacks of length zero ($\gamma$-shapes) is denoted by $\mathcal{S}_\gamma$. 
2.2 Some generating functions

In this paper we denote the ring of polynomials over a ring $R$ by $R[X]$ and the ring of formal power series $\sum_{n \geq 0} a_n X^n$ by $R[[X]]$. $R[[X]]$ is a local ring with maximal ideal $(X)$, i.e. any power series with nonzero constant term is invertible. A Puiseux series [Wall (2004)] is power series in fractional powers of $X$, i.e. $\sum_{n \geq 0} a_n X^{n/k}$ for some fixed $k \in \mathbb{N}$.

We denote the generating functions of a set of diagrams $D$ filtered by the number of arcs $D(z) = \sum_{n \geq 0} d(n) z^n$. Similarly, a generating function of diagrams filtered by the length of the backbone is written as $D(z) = \sum_{n \geq 0} d(n) z^n$. In particular, the generating functions of $\gamma$-matchings and $\tau$-canonical $\gamma$-structures are given by

$$H_\gamma(u) = \sum_{2n \geq 0} h_\gamma(n) u^n, \quad G_{\tau, \gamma}(z) = \sum_{n \geq 0} g_{\tau, \gamma}(n) z^n.$$ 

Let $H_\gamma(n, m) \supseteq S_\gamma(n, m)$ denote the collections of all $\gamma$-matchings and $\gamma$-shapes on $2n \geq 0$ vertices containing $m \geq 0$ 1-arcs with generating functions

$$H_\gamma(x, y) = \sum_{m, 2n \geq 0} h_\gamma(n, m) x^n y^m, \quad S_\gamma(x, y) = \sum_{m, 2n \geq 0} s_\gamma(n, m) x^n y^m,$$

where $h_\gamma(n, m) = s_\gamma(n, m) = 0$ if $2\gamma > n$ or if $m > n$.

Furthermore there is a natural projection $\vartheta$ from $\gamma$-matchings to $\gamma$-shapes defined by collapsing each non-empty stack onto a single arc

$$\vartheta: \mathcal{H}_\gamma \rightarrow \mathcal{S}_\gamma,$$

which is surjective and preserves irreducible shadows as well as the number of 1-arcs. $\vartheta$ restricts to a surjection

$$\vartheta: \sqcup_{n \geq 0} \mathcal{H}_\gamma(n, m) \rightarrow \sqcup_{n \geq 0} \mathcal{S}_\gamma(n, m),$$

which collapses each stack to an arc and preserves any irreducible shadow and also the number $m$ of 1-arcs.

3 Combinatorics of $\gamma$-matchings

In this section we study $\gamma$-matchings.

**Theorem 1** Let $R = \mathbb{Z}[u]$. Then the following assertions hold:

(a) the generating function of $\gamma$-matchings, $H_\gamma(u)$, satisfies

$$H_\gamma(u)^{-1} = 1 - \left( u H_\gamma(u) + H_\gamma(u)^{-1} \sum_{\gamma \leq g} I_g \left( \frac{u H_g^2(u)}{1 - u H_g(u)} \right) \right).$$

(1)

In particular, there exists a polynomial $P_\gamma(u, X) \in R[X]$ of degree $(12\gamma - 2)$, whose coefficients are sums of $I_g(z)$ coefficients, such that $P_\gamma(u, H_\gamma(u)) = 0$.

(b) eq. (1) determines $H_\gamma(u)$ uniquely.
First, a fixed irreducible shadow $\sigma$ is inflated into a $\mathcal{L}_\sigma$-diagram, second we pass to an $\mathcal{F}_\sigma$-diagram by inserting a nontrivial $\mathcal{L}_\sigma$-diagram in one of the $P$-intervals.

**Proof** We first prove (a). Let $\sigma$ be a fixed irreducible shadow of genus $g$ having $m$ arcs. Let $\mathcal{V}_\sigma$ be the set of diagrams, generated by concatenating and nesting $\sigma$.

Claim 1:

$$\mathcal{V}_\sigma(u) = (1 - \mathcal{V}_\sigma(u)^{-1}(u \mathcal{V}_\sigma(u)^2)^m)^{-1}.$$ 

To prove Claim 1 we consider a $\mathcal{V}_\sigma$-diagram. Clearly, its maximal arcs are contained in $t \geq 1$ copies of $\sigma$. These arcs induce exactly $(2m - 1)t$ $\sigma$-intervals, in each of which we find again an element of $\mathcal{V}_\sigma$, whence

$$\mathcal{V}_\sigma(u) = \sum_{t \geq 0} (u^m \mathcal{V}_\sigma(u)^{2m-1})^t$$

and Claim 1 follows.

Let $\mathcal{L}_\sigma$ be the set of diagrams having the fixed shape $\sigma$ obtained by inflating $\sigma$-arcs into stacks, or symbolically, $U \times \text{Seq}(U)$. Here $U$ and $R = \text{Seq}(U)$ denote the classes of arcs and sequences of arcs. Clearly, the associated generating function of $U \times R$ is $u(1 - u)^{-1}$.

Note that each $\mathcal{L}_\sigma$-diagram contains exactly $(2m - 1)$ $\sigma$-intervals and an arbitrary number of pairs of $P$-intervals. Let $\mathcal{F}_\sigma$ denote the set of diagrams generated by concatenating and nesting $\mathcal{L}_\sigma$-diagrams that contain no empty $P$-intervals. Let finally $\mathcal{W}_\sigma$ be the set of 1-canonical diagrams, having shapes in $\mathcal{F}_\sigma$.

Claim 2.

$$\mathcal{W}_\sigma(u)^{-1} = 1 - \mathcal{W}_\sigma(u)^{-1} \left( \frac{u}{1 - u} \frac{\mathcal{W}_\sigma^2(u)}{1 - \frac{u}{1 - u} (\mathcal{W}_\sigma^2(u) - 1)} \right)^m. \quad (2)$$

We shall construct $\mathcal{W}_\sigma$ using arcs, $U$, sequences of arcs, $R$, induced arcs, $N$, and sequence of induced arcs, $M$. The class $\mathcal{T}_\sigma$ is obtained by concatenating and nesting $\mathcal{L}_\sigma$-diagrams that do not contain any empty $P$-intervals, see Fig. 6, i.e. an arc together with at least one nontrivial $\mathcal{T}_\sigma$-diagram in either one or in both $P$-intervals

$$N = U \times \left( (\mathcal{T}_\sigma - 1) + (\mathcal{T}_\sigma - 1) + (\mathcal{T}_\sigma - 1)^2 \right) = U \times \left( \mathcal{T}_\sigma^2 - 1 \right).$$
Clearly, we have for a single induced arc \( N(u) = u F_\sigma(u)^2 - 1 \) and for a sequence of induced arcs, \( M = \text{Seq}(N) \), where

\[
N(u) = \frac{1}{1 - u F_\sigma(u)^2 - 1}.
\]

By construction, the maximal arcs of an \( F_\sigma \)-diagram coincide with those of its underlying \( V_\sigma \)-diagram. Therefore

\[
F_\sigma(u) = \sum_{t \geq 0} ((u \times M)^m) F_\sigma^2m - 1 \]t
\]

with generating function

\[
F_\sigma(u) = \sum_{t \geq 0} \left( \frac{u}{1 - u F_\sigma(u)^2 - 1} \right)^m F_\sigma(u)^2m - 1\]t.
(3)

Next we inflate the arcs of the \( F_\sigma \)-diagram into stacks, \( \mathcal{U} \times \mathcal{R} \). This inflation process generates \( W_\sigma \)-diagrams and any \( W_\sigma \)-diagram can be constructed from a unique fixed irreducible shadow \( \sigma \) of genus \( g \) with \( m \) arcs. We have

\[
W_\sigma(u) = \sum_{t \geq 0} \left( \frac{u}{1 - \frac{u}{W_\sigma(u)^2 - 1}} \right)^m W_\sigma(u)^2m - 1\]t.
(4)

whence Claim 2.

**Claim 3:** Let \( M \) be the set of irreducible shadows of genus \( g \leq \gamma \). Then

\[
W_M(u)^{-1} = 1 - \sum_{g \leq \gamma} \sum_{1 < m} i_g(m) W_M(u)^{-1} \left( \frac{u W_M^2(u)}{1 - u W_M(u)} \right)^m.
\]t
(5)

The maximal arcs of a \( V_M \)-structure, partition into the maximal arcs of \( t \) concatenated irreducible shadows \( \sigma_1, \ldots, \sigma_t \) and

\[
\sum_{\sigma_1, \ldots, \sigma_t} 1 = \left( \sum_{g \leq \gamma} \sum_{1 < m} i_g(m) \right)^t.
\]t
(6)

These maximal arcs induce exactly \( (2m - 1) t \) \( \sigma \)-intervals. In each \( \sigma \)-interval, we find again an element of \( V_M \). Thus for any \( \sigma_i \) having \( m \) arcs, we have \( V_M^{2m - 1} \), which leads to the term \( u^m V_M(u)^{2m - 1} \). It remains to sum over all \( t \), i.e. expressing all the decompositions of \( V_M \)-structures into concatenated, irreducible shadows and we obtain

\[
V_M(u) = \sum_{t \geq 0} \left( \sum_{g \leq \gamma} \sum_{m > 1} i_g(m) u^m V_M(u)^{2m - 1} \right)^t.
\]t
(7)

The passage to from \( V_M \) to \( L_M \) as well as that from \( L_M \) to \( F_M \) follows from Claim 2, whence

\[
F_M(u) = \sum_{t \geq 0} \left( \sum_{g \leq \gamma} \sum_{m > 1} i_g(m) F_M^{-1} \left( \frac{u F_M^2(u)}{1 - u F_M^2(u)} \right)^m \right)^t.
\]t
(8)
Here $F_M(u)^{-1}$ exists in $\mathbb{C}[[u]]$, having a nonzero constant term. Next we inflate the arcs of the $\mathcal{F}_M$-structure into stacks, obtaining

$$W_M(u)^{-1} = 1 - \sum_{g \leq \gamma} \sum_{1 < m} i_g(m) W_M(u)^{-1} \left( \frac{u W_M^2(u)}{1 - u (W_M^2(u))} \right)^m. \tag{9}$$

We next derive the functional equation for $H_\gamma(u)$ by incorporating noncrossing arcs. Since the maximal arcs composed of noncrossing arcs are exactly rainbows, the generating function of $\mathcal{F}_\gamma$-diagrams nested in a rainbow is given by $u H_\gamma(u)$. As in Claim 3 we conclude

$$H_\gamma(u)^{-1} = 1 - \sum_{g \leq \gamma} \left( u H_\gamma(u) + H_\gamma(u)^{-1} \sum_{m > 1} i_g(m) \vartheta(u)^m \right),$$

where

$$\vartheta(u) = \frac{u H_\gamma^2(u)}{1 - u H_\gamma^2(u)}.$$

Setting $w_u(X) = 1 - u X^2$, eq. (1) gives rise to the polynomial

$$P_\gamma(u, X) = w_u(X)^{\kappa_\gamma} (1 + X - u X^2) - \sum_{g \leq \gamma} w_u(X)^{\kappa_\gamma} I_g \left( \frac{u X^2}{w_u(X)} \right), \tag{10}$$

where $\kappa_\gamma = 6\gamma - 2$, $\deg(P_\gamma(u, X)) = (2 + 2\kappa_\gamma)$, $[X^{2 + 2\kappa_\gamma}] P_\gamma(u, X) = -u^{1 + \kappa_\gamma}$, and $P_\gamma(u, H_\gamma(u)) = 0$, whence (a).

It remains to prove (b). Since $M$ is the finite set of irreducible shadows of genus $g \leq \gamma$ and any such shadow has $2g \leq m \leq \kappa_\gamma$ arcs [Andersen et al. 2011], any $M$-shadow has $\leq \kappa_\gamma$ arcs. Setting $v(u) = 1 - u H_\gamma^2(u)$, eq. (1) implies

$$v(u)^{\kappa_\gamma} = H_\gamma(u) v(u)^{\kappa_\gamma} - u H_\gamma^2(u) v(u)^{\kappa_\gamma} - \sum_{g \leq \gamma} v(u)^{\kappa_\gamma} I_g \left( \frac{u H_\gamma^2(u)}{v(u)} \right),$$

and consequently

$$H_\gamma(u) = -H_\gamma(u) \sum_{i=1}^{\kappa_\gamma} \binom{\kappa_\gamma}{i} v(u)^{\kappa_\gamma - i} (v(u) - 1)^i + u H_\gamma^2(u) v(u)^{\kappa_\gamma} + v(u)^{\kappa_\gamma} \tag{11}$$

and

$$P_\gamma(u, H_\gamma(u)) = 0,$$
4 Analysis of 1- and 2-matchings

Let us begin recalling the following algebraic fact:

**Lemma 1** Let $R$ be an integral domain and $\varphi: R \rightarrow \overline{R}$ a homomorphism of $R$ into an integral domain $\overline{R}$. We consider the induced homomorphism $\varphi: R[X] \rightarrow \overline{R}[X]$. Suppose $f = \sum a_i X^i \in R[X]$ is primitive and $\overline{a_i} \neq 0$. Then

$$\overline{f} \text{ is irreducible } \implies f \text{ is irreducible.}$$

**Proof** Suppose $f$ is not irreducible in $R[X]$. Since $f$ is primitive, we then have necessarily a decomposition $f = gh$ where $g, h \in R[X]$ with $\deg(g) \geq 1$ and $\deg(h) \geq 1$. Applying $\varphi$ we obtain

$$\overline{f} = \overline{g} \overline{h}$$

and $\overline{a_i} \neq 0$ guarantees $\deg(g) = \deg(\overline{g}) \geq 1$ and $\deg(h) = \deg(\overline{h}) \geq 1$. Since $\overline{f}$ is by assumption irreducible, $\overline{g} \overline{h}$ leads to a contradiction. Consequently, $f$ has to be irreducible in $R[X]$.

**Lemma 2** $P_1(u, X)$ and $P_2(u, X)$ are irreducible in $R[X]$.

**Proof** According to Theorem 1 we have

$$P_\gamma(u, X) = w_u(X)^\gamma (-1 + X - uX^2) - \sum_{g \leq \gamma} w_u(X)^{\kappa_g} I_g \left( \frac{uX^2}{w_u(X)} \right),$$

where $\deg(P_\gamma(u, X)) = (2 + 2\kappa_\gamma)$, $P_\gamma(u, X) = -u^{1+\kappa_\gamma}$, and $P_\gamma(u, H_\gamma(u)) = 0$. In particular, for $\gamma = 1$:

$$P_1(u, X) = \sum_{j \leq 0} \sum_{g \leq 1} p_{1,j} X^{n-j}$$

$$= -u^5X^{10} + u^4X^9 + 3u^4X^8 - 4u^3X^7 - 2u^3X^6$$

$$+ 6u^2X^5 - 3u^2X^4 - 4uX^3 + 3uX^2 + X - 1.$$

For $\gamma = 2$ we obtain

$$P_2(u, X) = \sum_{j \leq 0} \sum_{g \leq 2} p_{2,j} X^{n-j}$$

$$= -u^{11}X^{22} + u^{10}X^{21} + 9u^{10}X^{20} - 10u^9X^{19} - 35u^9X^{18} + 45u^8X^{17}$$

$$+ 75u^7X^{16} - 120u^7X^{15} - 90u^7X^{14} + 210u^6X^{13} + 21u^6X^{12}$$

$$- 252u^5X^{11} - 16u^5X^{10} + 210u^4X^9 - 107u^4X^8 - 120u^3X^7$$

$$+ 75u^3X^6 + 45u^2X^5 - 35u^2X^4 - 10uX^3 + 9uX^2 + X - 1.$$

Let $\overline{R} = R/(u-1)$ and consider the ring homomorphism $R[X] \rightarrow \overline{R}[X]$ $X \mapsto X + (u-1)$. Clearly, $\overline{R} \cong \mathbb{Z}$, whence $R$ and $\overline{R}$ are both integral domains. Since $\frac{w_u(X)}{w_u(X)} = 1 - X^2$ in $\overline{R[X]} \cong \mathbb{Z}[X]$,

$$\overline{P}_\gamma(X) = (1 - X^2)^{\kappa_\gamma} (-1 + X - X^2) - \sum_{g \leq \gamma} (1 - X^2)^{\kappa_g} I_g \left( \frac{X^2}{(1 - X^2)} \right),$$

for $\gamma = 1$ and $\gamma = 2$. Then, we can conclude that $\overline{P}_1(X)$ and $\overline{P}_2(X)$ are irreducible in $\overline{R}[X]$.
is a primitive polynomial in \(\mathbb{Z}[X]\), where \(X^{2+2\gamma} \mathcal{T}_\gamma(X) = 1 \neq 0\). In particular, for \(\gamma = 1, 2\) we derive
\[
\mathcal{T}_1(X) = -X^{10} + X^9 + 3X^8 - 4X^7 - 2X^6 + 6X^5 - 3X^4 - 4X^3 + 3X^2 + X - 1
\]
and
\[
\mathcal{T}_2(X) = -X^{22} + X^{21} + 9X^{20} - 10X^{19} - 35X^{18} + 45X^{17} + 75X^{16} - 120X^{15} - 90X^{14} + 210X^{13} + 21X^{12} - 252X^{11} - 16X^{10} + 210X^9 - 107X^8 - 120X^7 + 75X^6 + 45X^5 - 35X^4 + 9X^2 + X - 1.
\]

Using Maple we can verify that \(\mathcal{T}_1(X), \mathcal{T}_2(X) \in \mathbb{Z}[X]\) are both irreducible.

Since \(P_1(u, X), P_2(u, X)\) are primitive and \(X^{2+2\gamma} \mathcal{T}_\gamma(X) = 1 \neq 0\), Lemma \[\text{1}\] implies that \(P_1(u, X), P_2(u, X)\) are irreducible in \(\mathbb{K}[X]\).

**Theorem 2** Let \(i = 1, 2\), and \(DP_i(u, X)\) be the discriminant of \(P_i(u, X)\) and let \(\mu_i\) denote the real dominant singularity of \(H_i(u)\).

(a) the dominant singularity \(\mu_i\) is unique and a root of \(DP_i(u, X)\),

(b) at \(\mu_i\) we have
\[
H_i(u) = \pi_i + \sum_{n \geq 1} a_{n,i} ((\mu_i - u)^{1/2})^n,
\]
where \(\pi_i\) is the root of minimal modulus of \(P_i(\mu_i, X)\) and \(a_{1,i} \neq 0\).

(c) the coefficients of \(H_i(u)\) are asymptotically given by
\[
[z^n]H_i(u) \sim k_i n^{-3/2} \left(\mu_i^{-1}\right)^n
\]
for some \(k_i > 0\), where \(\mu_1^{-1} \approx 8.28425\) and \(\mu_2^{-1} \approx 9.8724\), respectively.

**Proof** In order to prove (a), we observe that Lemma \[\text{2}\] allows us to employ Theorem 12.2.1 of [Hille (1962), pp. 103]. According to eq. (12.2.16) and eq. (12.2.17) of [Hille (1962)], the discriminant \(DP_i(u)\) can be expressed as
\[
DP_i(u) = (-1)^{\frac{1}{2}/4} n(n-1) \frac{1}{\rho_i,0(u)} \text{Res} \left[ P_i, \frac{\partial P_i}{\partial X} \right],
\]
where \(\text{Res} \left[ P_i, \frac{\partial P_i}{\partial X} \right]\) denotes the resultant of \(P_i\) and \(\frac{\partial P_i}{\partial X}\) as polynomials in \(X\). The resultant can be computed via a certain determinant [Hille (1962)] and we verify by direct computation that the dominant singularity is the root of minimal modulus of \(DP_i(z)\).

To prove (b), let \(\pi_i\) denote the unique real root of minimal modulus of \(P_i(\mu_i, X)\). Then
\[
R_i(u, X) = R_i(\mu_i - u, X - \pi_i) = P_i(u, X) = 0
\]
represents in the variables \((\mu_i - u)\) and \((X - \pi_i)\) a plane curve with a singularity at the origin, respectively. Puiseux’s Theorem [Wall (2004)] guarantees a solution of \(X - \pi_i\) in terms of a power series in fractional powers of \((\mu_i - u)\).
Claim. A solution of \( P_i(u, X) = 0 \) at \( u = \mu_i \) is given via a Puiseux series of the form

\[
X = \pi_i + \sum_{n \geq 1} a_{n,i} ((\mu_i - u)^{\frac{1}{2}})^n,
\]

where \( a_{1,i} \neq 0 \).

To prove the Claim, we use Lemma 2 and explicitly compute the coefficients \([u^1_i, X^0_i] R_i(u_i, X_i)\) and \([u^0_i, X^2_i] R(u_i, X_i)\). In particular,

\[
\begin{align*}
[u^1_i, X^0_i] R(u_i, X_i) &\neq 0 \\
[u^0_i, X^2_i] R(u_i, X_i) &\neq 0.
\end{align*}
\]

By construction, the curve \( R_i(u_i, X_i) = 0 \) has a singularity at the origin, whence

\[
\begin{align*}
[u^0_i, X^1_i] R(u_i, X_i) &= \frac{\partial R_i}{\partial X_i}(0,0) = 0.
\end{align*}
\]

Constructing the Puiseux series via the Newton polygon, we find the first exponent of \( u_1 \) to be \( \frac{1}{2} \) and furthermore

\[
\left[u^0_i, X^1_i\right] R_i(u_i, X_i) = a_{1,i}^2 + \left[u^1_i, X^0_i\right] R(u_i, X_i) = 0. \tag{17}
\]

Combining this observation with Theorem 2.1.1, pp 15-16, Wall (2004), we derive that there exists a power series in \( u_1/2 \) that satisfies \( P_i(u, X) = 0 \) at \( u = \mu_i \).

According to Theorem 1, \( H_i(z) \) is the unique solution of \( P_i(u, X) = 0 \), which ties the above Puiseux series to \( H_i(u) \), i.e.

\[
H_i(u) = \pi_i + \sum_{n \geq 1} a_{n,i} ((\mu_i - u)^{\frac{1}{2}})^n. \tag{18}
\]

Assertion (c) follows from eq. (18) as a straightforward application of the transfer theorem, Theorem VI.3, pp. 389 Flajolet and Sedgewick (2009).

5 Combinatorics of \( \gamma \)-diagrams

Lemma 3 For any \( \gamma \geq 1 \), we have

\[
S_\gamma(u, e) = \frac{1 + u}{1 + 2u - ue} H_\gamma \left( \frac{u(1 + u)}{(1 + 2u - ue)^2} \right). \tag{19}
\]

Proof We first prove

\[
H_\gamma(x, y) = \frac{1}{x + 1 - yx} H_\gamma \left( \frac{x}{(x + 1 - yx)^2} \right). \tag{20}
\]

Choose \( \xi \in \mathcal{H}_\gamma(s + 1, m + 1) \) and label one of its 1-chords. Since we can label any of the \((m + 1)\) 1-arcs of \( \xi \), \((m + 1)\) \( \mathbf{h}_\gamma(s + 1, m + 1) \) different such labeled linear arc diagrams arise. On the other hand, to produce \( \xi \) with this labeling, we can add one labeled 1-arc to an element of \( \mathcal{H}_\gamma(s, m + 1) \) by inserting a parallel copy of an existing 1-arc or by inserting a new labeled 1-arc in an element of \( \mathcal{H}_\gamma(s, m) \), where we may
only insert the 1-arc between two vertices not already forming a 1-arc. It follows that we have the recursion

\[(m + 1) h_\gamma(n + 1, m + 1) = (m + 1) h_\gamma(n, m + 1) + (2n + 1 - m) h_\gamma(n, m)\]

or equivalently the PDE

\[
\frac{\partial H_\gamma(x, y)}{\partial y} = x \frac{\partial H_\gamma(x, y)}{\partial x} + 2x^2 \frac{\partial H_\gamma(x, y)}{\partial x} + xH_\gamma(x, y) - xy \frac{\partial H_\gamma(x, y)}{\partial y},
\]

which is thus satisfied by \(H_\gamma(x, y)\).

On the other hand,

\[H_\gamma(x, y) = \frac{1}{x + 1 - xy} H_\gamma\left(x^{s}, (x + 1 - xy)^t\right)\]

is also a solution of eq. \((21)\), which specializes to \(H_\gamma(x) = H_\gamma^*(x, 1)\), and moreover, we have \(h_\gamma^*(n, m) = [x^n y^m] H_\gamma^*(x, y) = 0\), for \(m > n\). Indeed, the first assertion is easily verified directly, the specialization is obvious, and the fact that \(y\) only appears in the power series \(H_\gamma^*(x, y)\) in the form of products \(xy\) implies that \(h_\gamma^*(n, m) = 0\), for \(m > n\). Thus, the coefficients \(h_\gamma^*(n, m)\) satisfy the same recursion and initial conditions as \(h_\gamma(n, m)\), and hence by induction on \(n\), we conclude \(h_\gamma^*(n, m) = h_\gamma^*(m, n)\), for \(n, m \geq 0\). This proves that \(H_\gamma^*(x, y)\) indeed satisfies eq. \((20)\) as was claimed.

To complete the proof of eq. \((19)\), we use that the projection \(\vartheta\) is surjective and affects neither irreducible shadows nor the number of 1-arcs. Let us consider a fixed \(\gamma\)-shape, \(\lambda\), having \(s\) arcs, of which \(t\) are 1-arcs and the generating function \(H_\lambda^\gamma(x, y)\), counting \(\gamma\)-matchings that project into \(\lambda\). Then

\[H_\lambda^\gamma(x, y) = \left(\frac{x}{1 - x}\right)^s y^t\]

which shows that \(H_\lambda^\gamma(x, y)\) depends only on the total number of arcs and number of 1-arcs in \(\lambda\). Consequently,

\[H_\gamma(x, y) = \sum_{s \geq 0} \sum_{m = 0}^s s_\gamma(s, m) \left(\frac{x}{1 - x}\right)^s y^m = S_\gamma\left(\frac{x}{1 - x}, y\right).\]

Setting \(u = \frac{x}{1 - x}\), i.e., \(x = \frac{1 - u}{1 + u}\), and \(e = y\), we arrive at

\[S_\gamma(u, e) = \frac{1 + u}{1 + 2u - ue} H_\gamma\left(\frac{u(1 + u)}{(1 + 2u - ue)^2}\right),\]

as required.

**Lemma 4** Let \(\lambda\) be a fixed \(\gamma\)-shape with \(s \geq 1\) arcs and \(m \geq 0\) 1-arcs. Then the generating function of \(\tau\)-canonical \(\gamma\)-diagrams containing no 1-arc that have shape \(\lambda\) is given by

\[G_{\tau, \gamma}^\lambda(z) = (1 - z)^{-1} \left(\frac{z^{2\tau}}{(1 - z^2)(1 - z)^2 - (2z - z^2)z^{2\tau}}\right)^s z^m.
\]

In particular, \(G_{\tau, \gamma}^\lambda(z)\) depends only upon the number of arcs and 1-arcs in \(\lambda\).

Our main result about enumerating \(\tau\)-canonical \(\gamma\)-structures follows.
Table 1  The exponential growth rates of $\rho_{s,i}^{-1}$, for $1 \leq s, i \leq 2$.

| (s, i) | (1, 1) | (2, 1) | (1, 2) | (2, 2) |
|--------|--------|--------|--------|--------|
| $\rho_{s,i}^{-1}$ | 3.6005 | 2.2759 | 3.8846 | 2.3553 |

**Theorem 3**  Suppose $\gamma, \tau \geq 1$ and let $w_\tau(z) = \frac{(1 - z^{2\tau})^{-1}}{z^{2\tau} - z + 1}$. Then the generating function $G_{\tau, \gamma}(z)$ is algebraic and given by

$$G_{\tau, \gamma}(z) = \frac{1}{u_\tau(z)z^2 - z + 1} H_\gamma \left( \frac{u_\tau(z)z^2}{(u_\tau(z)z^2 - z + 1)^2} \right).$$  \hspace{1cm} (23)

**Proof**  Since each $\gamma$-diagram has a unique $\gamma$-shape, $\lambda$, having some number $m \geq 0$ of 1-arcs, we have

$$G_{\tau, \gamma}(z) = \sum_{m \geq 0} \sum_{\lambda \text{ shape having } m \text{ 1-arcs}} G_{\lambda, \tau, \gamma}(z).$$  \hspace{1cm} (24)

According to Lemma 3 $G_{\lambda, \tau, \gamma}(z)$ only depends on the number of arcs and 1-arcs of $\lambda$, and we can therefore express

$$G_{\tau, \gamma}(z) = \frac{1}{z - 1} S_\gamma \left( \frac{z^{2\tau}(1 - z)(1 - z^2)^{2} - (1 + z^2)^{2\tau}z^2}{(1 - z)^2 - (1 - z^2)^{2\tau}z^2 + z} \right)$$

$$= \frac{1}{(1 - z) + u_\tau(z)z^2} H_\gamma \left( \frac{z^2 u_\tau(z)}{((1 - z) + u_\tau(z)z^2)^2} \right),$$

using Lemma 3 in order to confirm eq. (26), where the second equality follows from direct computation. Let

$$\theta_\tau(z) = \frac{z^2 u_\tau(z)}{((1 - z) + u_\tau(z)z^2)^2}$$

denote the argument of $H_\gamma$ in this expression. By definition we have $\theta(z) \in \mathbb{C}(z)$. Since $\theta_\tau(0) = 0$ the composition $H_\gamma(\theta_\tau(z))$ is welldefined as a powerseries. Obviously, $P_\gamma(z, H_\gamma(z)) = 0$ guarantees $P_\gamma(\theta_\tau(z), H_\gamma(\theta_\tau(z))) = 0$. We have the following Hasse diagram of fields

$$\mathbb{C}(z, \theta_\tau(z), H_\gamma(\theta_\tau(z)))$$
$$\mathbb{C}(z, \theta_\tau(z))$$
$$\mathbb{C}(z)$$
$$\mathbb{C}(z, H_\gamma(z))$$
from which we immediately conclude that \( G_{\tau,\gamma}(z) \) is algebraic. Pringsheim’s Theorem [Flajolet and Sedgewick (2009)] guarantees that for any \( \gamma, \tau \geq 1 \), \( G_{\tau,\gamma}(z) \) has a dominant real singularity \( \rho_{\tau,\gamma} > 0 \).

According to Theorem 2 we have

\[
H_i(z) = \pi_i + \sum_{j \geq 1} a_{j,i} \left( (\mu_i - z)^{1/2} \right)^j \quad \text{and} \quad [z^n]H_i(z) \sim k_i n^{-3/2} \left( \mu_i^{-1} \right)^n.
\]

For \( \tau = 1, 2 \), we verify directly that \( \rho_{1,i} \) and \( \rho_{2,i} \) are the unique solutions of minimum modulus of \( \theta_1(z) = \mu_i \) and \( \theta_2(z) = \mu_i \). These solutions are strictly smaller than any other singularities of \( \theta_1(z) \) and \( \theta_2(z) \) and furthermore satisfy \( \theta'_1(\rho_{1,i}) \neq 0 \) as well as \( \theta'_2(\rho_{2,i}) \neq 0 \). It follows that \( \tilde{G}_{1,i}(z) \) and \( \tilde{G}_{2,i}(z) \) are governed by the supercritical paradigm [Flajolet and Sedgewick (2009)], which in turn implies

\[
[z^n]G_{s,i}(z) \sim k_{s,i} n^{-3/2} \left( \rho_{s,i}^{-1} \right)^n
\]

where \( s = 1, 2 \) and \( k_{s,i} \) is some positive constant.

Theorem 3 has its analogue for \( \tau \)-canonical, \( \gamma \)-diagrams containing 1-arcs. The asymptotic formula in case of \( \tau = 1, \gamma = 1 \),

\[
[z^n]G_{1,1}(z) \sim j_1 n^{-3/2} (\theta_{1,1}^{-1})^n
\]

is due to [Nebel and Weinberg (2011a)] who used the explicit grammar developed in [Reidys et al. (2011)] in order to obtain an algebraic equation for \( \tilde{G}_{1,1}(z) \).

**Corollary 1** Suppose \( \gamma, \tau \geq 1 \) and let \( u_\tau(z) = \frac{z^{\tau-1}}{2-z^{\tau}} \). Then the generating function of \( \tau \)-canonical \( \gamma \)-diagrams containing 1-arcs, \( \tilde{G}_{\tau,\gamma}(z) \), is algebraic and

\[
\tilde{G}_{\tau,\gamma}(z) = H_\gamma \left( \frac{u_\tau(z)z^2}{(1-z)^\tau} \right).
\]

In particular for \( \gamma = 1 \) we have

\[
[z^n]G_{1,1}(z) \sim j_1 n^{-3/2} (\theta_{1,1}^{-1})^n, \quad \text{and} \quad [z^n]G_{2,1}(z) \sim j_2 n^{-3/2} (\theta_{2,1}^{-1})^n
\]

for some constants \( j_1, j_2 \), where \( \theta_{1,1}^{-1} = 3.8782 \) and \( \theta_{2,1}^{-1} = 2.3361 \).

**Proof** Let \( \lambda \) be a fixed \( \gamma \)-shape with \( s \geq 1 \) arcs and \( m \geq 0 \) 1-arcs. Then the generating function of \( \tau \)-canonical \( \gamma \)-diagrams containing 1-arcs that have shape \( \lambda \) containing 1-arcs is given by

\[
\tilde{G}_{\tau,\gamma}(z) = (1-z)^{-1} \left( \frac{z^{2\tau}}{(1-z^2)(1-z)^2 - (2z - z^2)z^{2\tau}} \right)^s.
\]
Discussion

The symbolic approach based on $\gamma$-matchings allows not only to compute the generating function of canonical $\gamma$-structures. On the basis of Theorem 3 it is possible to obtain a plethora of statistics of $\gamma$-structures by means of combinatorial markers.

For instance, we can analogously compute the bivariate generating function of $\tau$ canonical $\gamma$-structures over $n$ vertices, containing exactly $m$ arcs, $A_{\tau,\gamma}(z, t)$ as

$$A_{\tau,\gamma}(z, t) = \frac{1}{u_\tau(z, t)z^2 - z + 1} \frac{u_\tau(z, t)z^2}{(u_\tau(z, t)z^2 - z + 1)^2}$$

where $u_\tau(z, t)$ is given by

$$u_\tau(z, t) = \frac{t(tz^2)^{\gamma-1}}{(t^2z^2 - tz^2 + 1)}.$$

This bivariate generating function is the key to obtain a central limit theorem for the distribution of arc-numbers in $\gamma$-structures Bender (1973) on the basis of Lévy-Cramér Theorem on limit distributions Feller (1991).

Statistical properties of $\gamma$-structures play a key role for quantifying algorithmic improvements via sparsifications Busch et al. (2008); Möhl et al. (2010); Wexler et al. (2007). The key property here is the polymer-zeta property Kabakcioglu and Stella (2008); Kafri et al. (2000) which states that the probability of an arc of length $\ell$ is bounded by $k\ell^c$, where $k$ is some positive constant and $c > 1$. Polymer-zeta stems from the theory of self-avoiding walks Vanderzande (1998) and has only been empirically established for the simplest class of RNA structures, namely those of genus zero. It turns out however, that the polymer-zeta property is genuinely a combinatorial property of a structure class. Moreover our results allow to quantify the effect of sparsifications of folding algorithms into $\gamma$-structures Andersen et al. (2011b); Huang and Reidys.

We finally remark that around 98% of RNA pseudoknot structures catalogued in databases are in fact canonical 1-structures. RNA pseudoknot structures like the HDV-virus exhibiting irreducible shadows of genus two are relatively rare.

Acknowledgements We want to thank Fenix W.D. Huang and Thomas J.X. Li for discussions and comments.

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