On the genus filtration of diagrams over two backbones

Benjamin M. M. Fu\textsuperscript{1}  Christian M. Reidys\textsuperscript{2}\textsuperscript{*}

Department of Mathematics and Computer Science,
University of Southern Denmark,
Campusvej 55, DK-5230
Odense M, Denmark

Email\textsuperscript{1}: benjaminfmm@imada.sdu.dk
number\textsuperscript{1}: 45-40485667

Email\textsuperscript{2}: duck@santafe.edu
number\textsuperscript{2}: 45-24409251
Fax\textsuperscript{2}: 45-65502325

\textsuperscript{2}Corresponding author.
Abstract

In this paper we compute the bivariate generating function of $\gamma$-matchings over two backbones, filtered by the number of arcs and the topological genus. $\gamma$-matchings over two backbones are chord-diagrams, obtained via concatenation and nesting of irreducible shapes of topological genus $\leq \gamma$. We show that the key information is contained in the polynomials counting these shapes and provide recursions that allow to compute the latter. In particular we give a bijection between such irreducible shapes over one and two backbones. We present two applications of our results. The first is concerned with RNA-RNA interaction structures, obtained from the $\gamma$-matchings via symbolic methods. We secondly show that, using analytic-combinatorial methods, the topological genus satisfies a central limit theorem.

Keywords: genus, generating function, recursion, matching, RNA interaction structure

1 Introduction

In this paper we study the generating function of diagrams over two backbones. These combinatorial structures are filtered by the number of arcs and also carry a natural topological filtration induced by the topological genus of their associated surface without boundary. Diagrams over two backbones play a central role in the context of folding algorithms of RNA-RNA interaction structures (Andersen et al., 2012a), i.e. complexes formed by two distinct RNA molecules. The key point here is that natural interaction struc-
tures are composed by irreducible “motifs” of small topological genus. It appears that therefore topological filtration offer a natural way of classifying such molecules.

It has been shown in (Andersen et al., 2012a) that for fixed topological genus, there exist only finitely many irreducible motifs, called irreducible shadows. This motivates the notion of $\gamma$-diagrams or $\gamma$-matchings, i.e. diagrams over two backbones composed by nesting such irreducible shadows of genus $\leq \gamma$. The algorithmic relevance of this finiteness lies in the fact that these shadows can be individually evaluated and measured. This allows to design RNA folding algorithms that go beyond associating a global penalty for crossing arcs, see for instance (Reidys et al., 2011), where this has been implemented for diagrams over one backbone.

Our main result is the bivariate generating function of $\gamma$-matchings over two backbones, filtered by the number of arcs and topological genus, $Q_\gamma(u, t)$, in Corollary (4.1). The latter is expressed as an algebraic expression involving the polynomials of irreducible shadows and the generating function of $\gamma$-matchings over one backbone $H_\gamma(u, t)$, computed in (Li and Reidys, 2012).

We finally discuss the implications of our results for RNA interaction structures (Huang et al., 2010, 2009). To this end we show how to derive the relevant generating functions via symbolic methods. In other words the biologically relevant structures can be constructed in a modular fashion (Reidys et al., 2010), resulting in a composition of power series. We furthermore present a central limit theorem that is a corollary of Theorem (3.1) and obtained via singularity analysis of $Q_\gamma(u, t)$ employing the quasi-powers
2 Some basic facts

2.1 Diagrams

A diagram is a labelled graph over the vertex set $[n] = \{1, ..., n\}$, in which each vertex has degree $\leq 3$. It can be represented by drawing its vertices in a horizontal line and its edges $(i, j)$, where $i < j$, in the upper half-plane. A backbone is a sequence of connected, consecutive integers contained in $[n]$. A diagram over $b$ backbones is a diagram together with a partition of $[n]$ into the $b$ backbones.

An interval $[i, i + 1]$ is called a gap if there exists a pair of subsequent backbones $B_1$ and $B_2$ such that $i(j)$ is the rightmost(leftmost) vertex of $B_1(B_2)$. The vertex $i$ is referred to as cut vertex.

We call backbone edges $B$-arcs and any other edge simply an arc. We shall distinguish exterior and interior arcs, where the former connect different backbones, see Fig. 1. Diagrams over multiple backbones without exterior arcs are simply disjoint unions of diagrams over one backbone.

The vertices and arcs of a diagram correspond to nucleotides and base pairs, respectively. For a diagram over $b$ backbones, the leftmost vertex of each backbone denotes the 5′ end of the RNA sequence, while the rightmost vertex denotes the 3′ end. A particular class of diagrams over two backbones represents RNA interaction structures (Huang et al., 2010, 2009). Interaction structures are oftentimes represented alternatively by drawing the two
Figure 1: LHS: a diagram over [13] with arcs \{(1, 6), (2, 5), (7, 8), (9, 13), (10, 12)\} and B-arc \{(1, 2), (2, 3)\}, \{(4, 5), (5, 6), (6, 7)\}, \{(8, 9), (9, 10), (10, 11), (11, 12), (12, 13)\}. RHS: a matching derived by removing the isolated vertices and relabelling the vertices.

backbones \(R\) and \(S\) on top of each other, where we label the vertices \(R_1\) to be the 5’ end of \(R\) and \(S_1\) to be the 3’ of \(S\).

Let us next specify first properties of diagrams representing RNA interactions structures. A vertex \(i\) is isolated if it is not incident to any arc (except of backbone arcs). A diagram is connected if and only if it is connected as a combinatorial graph (i.e. employing arcs as well as backbone arcs). A diagram that does not contain any isolated vertices is called a matching.

An interior stack of length \(\tau\) is a maximal sequence of “parallel” interior arcs, namely, \(((i, j), (i+1, j-1), \cdots, (i+\tau-1, j-\tau+1))\). An interior stack is \(\tau\)-canonical if it contains at least \(\tau\) interior arcs. Exterior stacks on \([i,j]\) and \(\tau\)-canonical exterior stacks are defined, accordingly.

A stack on \([i,j]\) of length \(k\) naturally induces \((k-1)\) pairs of intervals of the form \([i+l, i+l+1], [j-l-1, j-l]\) where \(0 \leq l \leq k-2\). Any of these \(2(k-1)\) intervals is referred to as a \(P\)-interval. A \(\tau\)-canonical interaction structure is a diagram in which each stack has length at least \(\tau\). Any interval other than a gap or \(P\)-interval is called a \(\sigma\)-interval. Clearly, a diagram over \([n]\), contains \((n-1)\) intervals and we distinguish three types: gap intervals,
$P$-intervals and $\sigma$-intervals, see Fig. 2. Let $\prec$ be the partial order on arcs given by $(i, j) \prec (i', j')$ if and only if $i' \leq i$ and $j \leq j'$. Any diagram has a unique set of maximal arcs. cf. Fig. 3.

2.2 Diagrams to topological surfaces

The specific drawing of a diagram $G$ in the plane determines a cyclic ordering on the half edges of the underlying graph incident on each vertex, thus
defining a corresponding fatgraph $G$. The collection of cyclic orderings is called fattening, one such ordering on the half-edges incident on each vertex. Each fatgraph $G$ determines an oriented surface $F(G)$, which is connected if $G$ is and has a topological genus $g(F(G))$. Clearly, $F(G)$ contains $G$ as a deformation retract and each $G$ represents a cell-complex (Massey, 1967) over $F(G)$.

A diagram $G$ hence determines a unique surface $F(G)$. Equivalence of simplicial and singular homology implies that Euler characteristic, $\chi$, and genus, $g$, of $F(G)$ are independent of the choice of the cell-complex $G$ and given by $\chi = v - e + r$ and $g = 1 - \frac{1}{2}\chi$, where $v, e, r$ are the number of discs, ribbons and boundary components in $G$.

Without affecting the topological type of the constructed surface, one may collapse each backbone to a single vertex with the induced fattening called the polygonal model of the RNA. It is the orientation of each backbone from the 5’ end to the 3’ end that allows to transform the fatgraph of an RNA-structure or RNA-interaction structure into a fatgraph with one or two vertices. This backbone-collapse preserves orientation, Euler characteristic and genus, by construction. It is reversible by inflating each vertex to form a backbone. Using the collapsed fatgraph representation, we see that for a connected diagram over $b$ backbones, the genus $g$ of the surface is determined by the number $n$ of arcs and the number $r$ of boundary components, namely, $2 - 2g - r = v - e = b - n$.

Diagrams over one and two backbones are related by gluing, i.e., we have
the mapping
\[ \alpha : \mathcal{E} \to \mathcal{D}, \]
where \( \alpha(E) \) is obtained by keeping all arcs in \( E \) and connecting the 3’ end of \( R \) and the 5’ end of \( S \). Furthermore, given two diagrams over two backbones, \( E_1, E_2 \in \mathcal{E} \), we can insert \( E_2 \) into the gap of \( E_1 \) via concatenating the backbones \( R_2 \) and \( R_1 \) and \( S_1, S_2 \) preserving orientation. This composition is again a diagram over two backbones, \( E_1 \bullet E_2 \), i.e. we have
\[ \mu : \mathcal{E} \times \mathcal{E} \to \mathcal{E}, \quad \mu(E_1, E_2) = E_1 \bullet E_2. \]
It is straightforward to see that \( \bullet \) is an associative product with unit given by the diagram over two empty backbones. The product \( \bullet \) is not commutative.

### 2.3 Shadows

A shadow is a diagram with no non-crossing arcs or isolated vertices in which each stack has size one. The shadow of a diagram is obtained by removing all non-crossing arcs, deleting all isolated vertices and collapsing each induced stack to a single arc. We shall denote the shadow of a diagram \( X \) by \( sd(X) \), note that \( sd^2(X) = sd(X) \). Projecting into the shadow does not affect genus, i.e., \( g(X) = g(sd(X)) \). In case there are no crossing arcs, \( sd(X) \) becomes an empty diagram on the same number of backbones as \( X \). By definition, any empty backbone contributes one boundary component. For example, for a diagram \( X \) over \( b \) backbones that contains no crossing arcs, \( sd(X) \) is a sequence of \( b \) empty backbones with \( b \) boundary components.

In the case of the shadows over two backbones, We distinguish the shadows by type \( A \) and type \( B \). \( A \)-shadows are those where both backbones
are contained in one boundary component, all others are referred to as $B$-shadows. Let $A_{g,m}$ denote the class of all the $A$-shadows of genus $g$ with $m$ arcs, and let $B_{g,m}$ denote the class of all the $B$-shadows of genus $g$ with $m$ arcs.

Given a shadow over one backbone, we select any of its arcs, $a$. We inflate $a$ into a stack of size two and call the resulting diagram a $d$-shadow. Let $I_{g,m}$ be the class of shadows over one backbone having genus $g$ and $m$ arcs and $D_{g,m+1}$ the class of the $d$-shadows, having $(m + 1)$ arcs, induced by $I_{g,m}$.

**Lemma 2.1.** There is a bijection

$$\alpha: A_{g,m} \cup B_{g-1,m} \rightarrow I_{g,m} \cup D_{g,m}.$$  

**Proof.** Given a genus $g$ shadow $s$ over two backbones we glue via $\alpha$ and mark the corresponding location where we glued. This generates either a shadow over one backbone or a $d$-shadow with a mark, respectively. Furthermore, this operation is invertible. Namely, we can simply cut the backbone at the marked point.

It thus remains to consider the genera of the shadows involved. Suppose first $s$ is a $A$-shadow, we will show that then $\alpha$ does not change genus. Indeed, gluing an $A$-shadow always splits a boundary component, whence the number of boundary components increases by one. Evidently, the number of backbones decreases by one while the number of arcs does not change. Consequently, since $g' = (2 + n - (r + 1) - (b - 1))/2 = g$, the genus does not change.

Suppose next $s$ is a $B$-shadow. Then gluing will merge two boundary components. Thus, the number of boundary components decreases by one
and \( g' = (2 + n - (r - 1) - (b - 1))/2 = g + 1 \) shows that the genus increases by one. As a result,

\[
\alpha : A_{g,m} \cup B_{g-1,m} \longrightarrow \mathcal{I}_{g,m} \cup \mathcal{D}_{g,m},
\]

is a bijection as stipulated.

We furthermore have

**Theorem 2.2.** [Andersen et al., 2012a]. A shadow of genus \( g \geq 0 \) over two backbones has the following properties:

(a) For \( g \geq 1 \) it contains at least \( (2g + 1) \) and at most \( (6(g + 1) - 2) \) arcs; a shadow of genus 0 has at least 2 and at most 4 arcs. In particular, the set of such shadows is finite;

(b) There exists at least one shadow over two backbones with genus \( g \) containing exactly \( \ell \) arcs, where

\[
\ell = \begin{cases} 
(2g + 1) \leq \ell \leq 6(g + 1) - 2 & \text{for } g \geq 1, \\
2 \leq \ell \leq 4 & \text{for } g = 0.
\end{cases}
\]

(1)

**Proof.** First we recall an observation about shadows over one backbone [Reidys et al., 2011]. Shadows of genus \( g \geq 1 \) over one backbone have the following properties:

Claim 1.

(a) A shadow of genus \( g \) contains at least \( 2g \) and at most \( (6g - 2) \) arcs. In particular, for fixed \( g \) there are only finitely many shadows;

(b) For any \( 2g \leq \ell \leq 6g - 2 \), there exists a shadow of genus \( g \) containing exactly \( \ell \) arcs.
To prove this we note that if there is more than one boundary component, then there must be an arc with two different boundary components on its two sides. Removing this arc decreases \( r \) by exactly one while preserving \( g \) since the number of arcs is given by \( n = 2g + r - 1 \). Furthermore, if there are \( \nu_\ell \) boundary components of length \( \ell \) in the polygonal model, then
\[
2n = \sum_\ell \ell \nu_\ell \quad \text{since each side of each arc is traversed once by the boundary.}
\]
For a shadow, \( \nu_1 = 0 \) by definition, and \( \nu_2 \leq 1 \) as one sees directly. Therefore
\[
2n = \sum_\ell \ell \nu_\ell \geq 3(r - 1) + 2, \quad \text{so} \quad 2n = 4g + 2r - 2 \geq 3r - 1, \quad i.e., \quad 4g - 1 \geq r.
\]
Thus, we have \( n = 2g + (4g - 1) - 1 = 6g - 2 \), i.e., any shadow can contain at most \((6g - 2)\) arcs. The lower bound \( 2g \) follows directly from \( n = 2g + r - 1 \), since \( r \geq 1 \).

Let \( S_{2g} \) be a shadow containing \( 2g \) mutually crossing arcs, i.e., each arc crosses any of the remaining \((2g - 1)\) arcs. \( S_{2g} \) has genus \( g \) and contains a unique boundary component of length \( 4g \), i.e., traversing \( 4g \) non-backbone arcs counted with multiplicity. We construct a new shadow \( S_{2g+1} \) of genus \( g \) containing \((2g + 1)\) arcs, by inserting an arc crossing into \( S_{2g} \) from the \( 5' \) end of \( S_{2g} \) such that the boundary component in \( S_{2g} \) splits into one boundary component of length \( 3 \) and another of length \( 4g + 2 - 3 = 4g - 1 \). The latter becomes the first boundary component of \( S_{2g+1} \). The newly inserted arc is by construction crossing, splits a boundary component and preserves genus. We now prove the assertion by induction of the number of inserted arcs. By the induction hypothesis, there exists a shadow \( S_{2g+i} \) of genus \( g \) having \((2g + i)\) arcs, whose first boundary component has length \((4g - i)\). Again, we insert a crossing arc as described above thereby splitting the first
boundary component into one of length 3 and the other of length \((4g-(i+1))\).

After \(i = 4g-2\) such insertions, we arrive at a shadow whose first boundary component has length 2 while all other boundary components have length 3. Accordingly, there exists a set \(\{S_{2g}, S_{2g+1}, \ldots, S_{2g+(4g-2)}\}\) of shadows all having genus \(g\), where each \(S_j\) contains \(j\) arcs.

We finally observe that a shadow of genus \(g = 0\) over two backbones has at least 2 arcs, while the maximum number of arcs contained in such a shadow is given by \(6(0+1)-2 = 4\). For \(g \geq 1\), it is impossible to cut a shadow of genus \(g\) having \(2g\) arcs and keep the genus. Thus the shadow of genus \(g\) over two backbones has at least \((2g+1)\) arcs. By Lemma (2.1), We can always map an arbitrary shadow over two backbones of genus \(g\) via \(\alpha\) into a shadow over one backbone (of genus \(g\) or \((g+1)\)) or a \(d\)-shadow (of genus \(g\)). Claim 1 guarantees that there are only finitely many such shadows and \(d\)-shadows, and the theorem follows.

\(\square\)

### 2.4 Irreducibility

A diagram \(E\) over \(b\) backbones is called **irreducible**, if it is connected and for any two arcs, \(\alpha_1, \alpha_k\), there exists a sequence of arcs

\[
(\alpha_1, \alpha_2, \ldots, \alpha_{k-1}, \alpha_k),
\]

such that \((\alpha_i, \alpha_{i+1})\) are crossing. As proved in ([Andersen et al., 2012a](#)), we have the following corollary of Theorem (2.2).

**Corollary 2.3.** An irreducible shadow having genus \(g = 0\) over two backbones contains at least 2 and at most 4 arcs. For any \(\ell \leq \ell \leq 4\), there exists an
irreducible shadow of genus $g = 0$ over two backbones having exactly $\ell$ arcs.

An irreducible shadow having genus $g \geq 1$ has the following properties:

(a) Every irreducible shadow with genus $g$ over two backbones contains at least $(2g + 1)$ and at most $(6(g + 1) - 2)$ arcs;

(b) For arbitrary genus $g$ and any $2g + 1 \leq \ell \leq 6g - 2$, there exists an irreducible shadow of genus $g$ over one backbone having exactly $\ell$ arcs.

Let $X$ be a diagram. We call $S'$ an irreducible shadow of $X$ (irreducible $X$-shadow) if $S'$ is an irreducible shadow and any arc in $S'$ is contained in $X$. $S'$ is a $(g, b, m)$-shadow if $S'$ is a diagram over $b$ backbones having genus $g$ and $m$ arcs. The set of irreducible $(g, b, m)$-shadows is denoted by $I_{g, b, m}$. Let $I_{g, b} = \bigcup_m I_{g, b, m}$.

According to Corollary (2.3), the generating function

$$I_{g, b}(u) = \sum i_{g, b}(m)u^m$$

of the combinatorial class $I_{g, b}$ is in fact a polynomial.

The generating polynomials for $I_{g, b}(u)$ for $0 \leq g \leq 1$ and $1 \leq b \leq 2$ are

- $I_{1,1}(u) = u^2 + 2u^3 + u^4$,
- $I_{2,1}(u) = 17u^4 + 160u^5 + 566u^6 + 1004u^7 + 961u^8 + 476u^9 + 96u^{10}$,
- $I_{0,2}(u) = 3u^2 + 3u^3 + u^4$,
- $I_{1,2}(u) = 11u^3 + 137u^4 + 656u^5 + 1520u^6 + 1951u^7 + 1436u^8 + 572u^9 + 96u^{10}$.

A diagram is a $\gamma$-structure if it is connected and all its irreducible shadows have genus at most $\gamma$. A $\gamma$-structure is called $\tau$-canonical if every stack in
the structure have at least $\tau$ arcs. A $\gamma$-matching is a $\gamma$-structure without isolated vertices. The combinatorial class of $\gamma$-matchings over one backbone is denoted by $\mathcal{H}_\gamma$ with generating function $H_\gamma(u)$. We have

**Theorem 2.4.** ([Han et al., 2012]) Let $R = \mathbb{Z}[u]$. Then $H_\gamma(u)$, satisfies

$$H_\gamma(u)^{-1} = 1 - \left(uH_\gamma(u) + H_\gamma^{-1}(u) \sum_{g \leq \gamma} I_{g,1} \left( \frac{uH_\gamma^2(u)}{1 - uH_\gamma^2(u)} \right) \right). \tag{2}$$

Furthermore, eq. (2) determines $H_\gamma(u)$ uniquely. In case of $\gamma = 1$, the coefficients of $H_1(u)$ are asymptotically given by

$$[z^n]H_1(u) \sim k n^{-3/2} \left(\rho^{-1}\right)^n, \tag{3}$$

in which $k$ is some positive constant and $\rho^{-1} \approx 8.28425$.

The combinatorial classes of $\gamma$-matchings over two backbones is denoted by $\mathcal{Q}_\gamma$. We call $\gamma$-structures over two backbones also $\gamma$-interaction structures. Then

**Theorem 2.5.** ([Qin and Reidys, 2012]) The generating function of $\gamma$-matchings over two backbones, $\mathcal{Q}_\gamma(u)$, satisfies

$$Q_\gamma(u) = \frac{H_\gamma^2(u) \left( uH_\gamma^2(u) + \sum_{g \leq \gamma} I_{g,2} \left( \frac{uH_\gamma^2(u)}{1 - uH_\gamma^2(u)} \right) \right)}{1 - uH_\gamma^2(u) - \sum_{g \leq \gamma} I_{g,2} \left( \frac{uH_\gamma^2(u)}{1 - u} \right)} \tag{4}$$

For $\gamma = 0, 1$ the coefficients of $\mathcal{Q}_\gamma(u)$ are asymptotically given by $[u^n]Q_\gamma(u) \sim k_\gamma (\delta_\gamma^{-1})^n$ for some constant $k_\gamma > 0$. In particular, $\delta_0^{-1} \approx 5.4252$ and $\delta_1^{-1} \approx 8.7266$. 

14
3 Irreducible shadows and genus filtration

For shadows and matchings over one backbone, we have the bivariate generating function of irreducible shadows filtered by genus $g$ and arcs number $n$ denoted by

$$I(u, t) = \sum_{g \geq 1} I_g(u)t^g = \sum_{g \geq 1} \sum_{n=2g}^{6g-2} i_g(n)u^n t^g.$$  \hspace{1cm} (5)

We denote the class of all the matchings over 1-backbone by $C$. Let furthermore $c_g(n)$ denote the number of matchings of genus $g$ with $n$ arcs and

$$C_g(u) = \sum_{n \geq 2g} c_g(n)u^n.$$ \hspace{1cm} (6)

Then the bivariate generating function of matchings filtered by genus $g$ and arc number $n$ is

$$C(u, t) = \sum_{g \geq 0} C_g(u)t^g = \sum_{g \geq 0} \sum_{n \geq 2g} c_g(n)u^n t^g.$$ \hspace{1cm} (7)

In case of two backbones, by distinguishing $A$-shadows and $B$-shadows. We denote the bivariate generating polynomials, by $I_{2,A}(u, t)$ and $I_{2,B}(u, t)$:

$$I_{2,A}(u, t) = \sum_{g \geq 0} I_{2,A_g}(u)t^g = \sum_{g \geq 1} \sum_{n=2g+1}^{6(g+1)-2} i_{2,A_g}(n)u^n t^g + \sum_{n=2}^{n=4} i_{2,A_0}(n)u^n,$$ \hspace{1cm} (8)

$$I_{2,B}(u, t) = \sum_{g \geq 0} I_{2,B_g}(u)t^g = \sum_{g \geq 1} \sum_{n=2g+1}^{6(g+1)-2} i_{2,B_g}(n)u^n t^g + \sum_{n=2}^{n=4} i_{2,B_0}(n)u^n.$$ \hspace{1cm} (9)

We furthermore denote the set of all the matchings over 2-backbones by $Q$ and by $q_g(n)$ the number of matchings over two backbones of genus $g$ with $n$ arcs. Then let

$$Q_g(u) = \begin{cases} \sum_{n \geq 2g+1} q_g(n)u^n & \text{for } g \geq 1, \\ \sum_{n \geq 2} q_0(n)u^n & \text{for } g = 0. \end{cases}$$
The bivariate generating function of matchings over two backbones filtered by genus \( g \) and arc number \( n \) is \( Q(u, t) = \sum_{g \geq 0} Q_g(u) t^g \). The central observation is that \( Q(u, t) \) can be expressed via irreducible shadows as follows:

**Theorem 3.1.** The generating functions \( Q(u, t), C(u, t), I_{2,A}(u, t) \) and \( I_{2,B}(u, t) \) satisfy

\[
Q(u, t) = \frac{C(u, t)^2 \left( I_{2,A} + I_{2,B} - t I_{2,B}^2 - I_{2,A} I_{2,B} + u C(u, t)^2 (1 - I_{2,B}) \right)}{(1 - t I_{2,B}) (1 - u C(u, t)^2 - I_{2,A} - t I_{2,B})},
\]

where \( I_{2,A} = I_{2,A} \left( \frac{u C(u, t)^2}{1 - u C(u, t)^2}, t \right) \) and \( I_{2,B} = I_{2,B} \left( \frac{u C(u, t)^2}{1 - u C(u, t)^2}, t \right) \).

**Proof.** Let \( s \) be an arbitrary \( Q \)-matching. Consider the set of irreducible shadows which contain at least one exterior \( s \)-arc, \( Sh_2(s) \). There exists exactly one element in \( Sh_2(s) \), consisting of maximal arcs, i.e. all elements in \( Sh_2(s) \) are nested via •-product.

Our first goal shall be the computation of the generating function of two backbone matchings containing exactly \( p \), distinct, nested shadows, \( Q_p(u, t) \).

**Claim 0.** \( Q_0(u, t) = \frac{u C(u, t)^2}{1 - u C(u, t)^2} \).

To prove Claim 0, we note that here the two backbones are connected by at least 1 exterior arc that does not belong to any irreducible 2-shadow. If there are \( l \geq 1 \) such exterior arcs, these form an exterior stack. Let \( s^* \) denote the particular \( A_l \)-matching over \([2l]\) consisting of \( l \) non-crossing exterior arcs. Any \( A_l \)-matching, \( s \), can be obtained from \( s^* \) in three steps, see Fig. 4:

1. (I) Insert non-empty 1-backbone matchings into at least one of the two intervals of each pair of \([(i, i + 1), [2l - i, 2l - i + 1])\). Since there are \((l - 1)\) such intervals in \( s^* \), we obtain \( U^l \times (C^2 - E)^{l-1} \);
Figure 4: (a) is a $A_3$ matching, consisting of 3 exterior arcs. Step I: Insert non-empty matchings into the $P$ intervals. Step II: Inflate each exterior arc to a stack. Step III: Concatenation on each end of the (two) backbones.

(II) Inflate each exterior arc in the derived matching into an exterior stack. Since there are in total $l$ exterior arcs after Step (I), we obtain $\mathcal{N}_l = (\mathcal{U} \times \text{SEQ} (\mathcal{U}))^l \times (\mathcal{C}^2 - \mathcal{E})^{l-1}$, where $\text{SEQ} (\mathcal{U}) = \mathcal{E} + \mathcal{U} + \mathcal{U}^2 + \cdots$;

(III) Concatenate each end of the (two) backbones with a (possible empty) 1-backbone matching, i.e. $\mathcal{C}^4 \times \mathcal{N}_l$. 

17
Accordingly,

$$\mathcal{A}_l = \mathcal{C}^4 \times (\mathcal{U} \times \text{SEQ}(\mathcal{U}))^l \times (\mathcal{C}^2 - \mathcal{E})^{l-1},$$

for some $l \geq 1$. If the matching contains no 2-backbone shadows, in step (I) and (III) the genus increases by the genus of the added 1-backbone matchings. In step (II) the genus does not change. Then by summing over all $l \geq 1$:

$$Q_0(u, t) = \frac{u \mathcal{C}(u, t)^4}{1 - u \mathcal{C}(u, t)^2},$$

as claimed.

**Claim 1.**

$$Q_1(u, t) = \mathcal{I}_{2,A}(u \mathcal{C}(u, t)^2, t) \frac{(\mathcal{A}(u, t) + \mathcal{C}(u, t)^2)^2}{\mathcal{C}(u, t)^2} + \mathcal{I}_{2,B}(u \mathcal{C}(u, t)^2, t) \frac{t \mathcal{A}(u, t)^2 + 2t \mathcal{A}(u, t) \mathcal{C}(u, t)^2 + \mathcal{C}(u, t)^4}{\mathcal{C}(u, t)^2}.$$  

Let $\phi$ be a fixed irreducible shadow of genus $g$, having $m$ arcs and let $\mathcal{W}_\phi$ be the set of matchings over two backbones, $s$, that contain only $\phi$ as shadow. In the following we shall construct such $\mathcal{W}_\phi$-matchings, see Fig. 5. Let $\mathcal{A} \times \mathcal{X}$ be the class of all possible diagrams such that $d \in \mathcal{A} \times \mathcal{X}$ is either an $A$-matching or a $X$-matching, where $X$-matching is $\mathcal{C} \times \mathcal{C}$. That is, $\mathcal{A} \times \mathcal{X} = \mathcal{A} + \mathcal{X}$.

**Step 1**: Inflate each arc in $\phi$ into a sequence of induced exterior arcs, i.e. an exterior arc together with at least one non-trivial matching over one backbone in either one or in both $P$-intervals, i.e.

$$\mathcal{N} = \mathcal{R} \times ((\mathcal{C} - 1) + (\mathcal{C} - 1) + (\mathcal{C} - 1)^2) = \mathcal{R} \times (\mathcal{C}^2 - 1).$$ (14)
Figure 5: (a) is an irreducible shadow of genus 0 with 2 arcs; step 1: Inflate each arc in the shadow to a sequence of induced exterior arcs (red arcs); step 2: Inflate each exterior arc to a stack (blue arcs); step 3: Insert a $C$-matching into the 2 $\sigma$-intervals (green arcs).

Clearly, we have $N(u, t) = u \left( C(u, t)^2 - 1 \right)$ (for a single induced exterior arc). Furthermore, for a sequence of induced arcs $M = SEQ(N)$, we have

$$M(u, t) = \frac{1}{1 - u \left( C(u, t)^2 - 1 \right)}. \quad (15)$$

Inflating each exterior arc into a sequence of induced arcs, $R^m \times M^m$, leads to

$$u^m M(u, t)^m = \left( \frac{u}{1 - u \left( C(u, t)^2 - 1 \right)} \right)^m. \quad (16)$$
Step 2: Inflate each exterior arc into a stack. The corresponding generating function is
\[
\left( u \frac{1}{1 - u} \frac{1}{C(u, t)^2 - 1} \right)^m = \left( u \frac{1}{1 - uC(u, t)^2} \right)^m .
\] (17)

Step 3: Insert a \( C \)-matching into the respective \((2m - 2)\) \( \sigma \)-intervals of \( \phi \). The corresponding generating function is \( C(u, t)^{2m-2} \).

We thus arrive at
\[
t^g \left( u \frac{1}{1 - uC(u, t)^2} \right)^m C(u, t)^{2m-2} .
\] (18)

Next we add \( AX \) to the two termini, considering the four cases \( A \cdot \phi \cdot A \), \( \phi \cdot X \cdot A \), \( X \cdot \phi \cdot X \), and \( X \cdot \phi \cdot X \), see Fig. 6.

Figure 6: The four cases of adding \( AX \).

Lemma 1 in (Andersen et al., 2012a) allows to compute genus: if \( \phi \) is a \( A \)-shadow, the genus of the structure is just the sum of the substructure genera. In case of \( \phi \) being a \( B \)-shadow, the genus contribution is \((g(\phi_B) + 1)\)
Figure 7: A-shadow (a): if an exterior arc is added, the genus does not change. B-shadow (b), if an exterior arc is added, the genus increases by 1.

if there exist exterior arcs not contained in the shadow. However, if there are no such exterior arcs, the genus contribution is $g(\phi_B)$, see Fig. [7]

Accordingly, the generating function of $\mathcal{W}_{\phi_A}$ is

$$
\mathcal{W}_{\phi_A}(u, t) = t^g \left( \frac{u}{1 - uC(u,t)^2} \right)^m C(u,t)^{2m-2} (A(u,t) + C(u,t)^2)^2. \quad (19)
$$

For $\phi$ being of type $B$ we obtain

$$
\mathcal{W}_{\phi_B}(u, t) = t^g \left( \frac{u}{1 - uC(u,t)^2} \right)^m C(u,t)^{2m-2} (tA(u,t)^2 + 2tA(u,t)C(u,t)^2 + C(u,t)^4).
$$

(20)

Our above arguments only depend on the number of $\phi$-arcs and the type of $\phi$. Thus we have for any other irreducible shadow $\varrho$ of genus $g$ over two backbones having the same number of arcs and the same type, $\mathcal{W}_{\phi}(u, t) = \mathcal{W}_{\varrho}(u, t)$. Consequently we arrive at

$$
\mathcal{Q}_1(u, t) = \sum_{g \geq 0} \left( \sum_{\phi \in A} \mathcal{W}_{\phi_A}(u, t) + \sum_{\phi \in B} \mathcal{W}_{\phi_B}(u, t) \right), \quad (21)
$$

and

21
\( Q_1(u, t) = \sum_{g,m} \left[ i_{2,A_2}(m)t^g \left( \frac{u}{1-uC(u,t)^2} \right)^m \right. \)  
\( C(u, t)^{2m-2} \left( A(u, t) + C(u, t)^2 \right)^2 + \left. i_{2,B_2}(m)t^g \left( \frac{u}{1-uC(u,t)^2} \right)^m \right. \)  
\( C(u, t)^{2m-2} \left[ tA(u, t)^2 + 2 tA(u, t)C(u, t)^2 + C(u, t)^4 \right] \)  
\( = I_{2,A} \left( \frac{uC(u, t)^2}{1-uC(u, t)^2}, t \right) \left( A(u, t) + C(u, t)^2 \right)^2 \)  
\( + I_{2,B} \left( \frac{uC(u, t)^2}{1-uC(u, t)^2}, t \right) \left( tA(u, t)^2 + 2 tA(u, t)C(u, t)^2 + C(u, t)^4 \right) \)  

as claimed.

Suppose next we have \( p \geq 2 \). We shall distinguish three scenarios:

- \( s \) contains exactly \( m > 0 \) \( A \)-shadows and \( n \) \( B \)-shadows, where \( m + n = p \). Then the genus contribution is:
  \( \sum_{i=1}^{m} g(A_i) + \sum_{i=1}^{n} (g(B_i) + 1) \),

- \( s \) contains no \( A \)-shadows, but there exist some exterior arcs that do not belong to \( B \)-shadows. Then genus contribution is \( \sum_{i=1}^{p} (g(B_i) + 1) \),

- The exterior arcs of the matching are exclusively generated by \( B \)-shadows, see Fig. \( \text{S} \). Then the exterior arcs of \( s \) can be decomposed in to \( p \) shadows of type \( B \), each of these has genus \( g_j \). Their corresponding genus is \( \sum_{j=1}^{p} (g_j + 1) - 1 \).

Let \( \mathcal{T} \) denote the combinatorial class of all the matchings over two backbones whose genus is given by \( g = \sum g_A + \sum (g_B + 1) + \sum g_C \), where \( \sum g_A \) is
the sum of the genera of all $A$-shadows, $\sum (g_B + 1)$ is the sum of the genera of all $B$-shadows plus one, respectively. $\sum g_C$ is the sum of all the genera of inserted $C$-matchings. That is $T$ neglects the genus decrease by 1 when encountering the pure $B$-shadow case. Let $T_p$ denote the class of these matchings that contain $p$ nested shadows and $T_p(u, t)$ the corresponding generating function.

Claim 2.1

\[ T_1(u, t) = \left[ I_{2,A} \left( \frac{uC(u, t)^2}{1 - uC(u, t)^2}, t \right) + t \cdot I_{2,B} \left( \frac{uC(u, t)^2}{1 - uC(u, t)^2}, t \right) \right] \cdot \frac{(A(u, t) + C(u, t)^2)^2}{C(u, t)^2}. \]  

(24)

The proof is analogous to that of Claim 1, the only difference emerging when adding the class $\mathcal{AX}$: for $B$-shadows there is no need to distinguish the cases $\mathcal{A}$ and $\mathcal{X}$.

Claim 2.2 For $p \geq 2$, we have

\[ T_p(u, t) = T_{p-1}(u, t) \cdot \left[ I_{2,A} \left( \frac{uC(u, t)^2}{1 - uC(u, t)^2}, t \right) + t \cdot I_{2,B} \left( \frac{uC(u, t)^2}{1 - uC(u, t)^2}, t \right) \right] \cdot \frac{(A(u, t) + C(u, t)^2)}{C(u, t)^2}. \]  

(25)
To prove Claim 2.2, let $\hat{T}_p$ denote the subset of $T$-matchings $s$ whose maximal arcs constitute an irreducible shadow $sh$ in $Sh_2(s)$. Any $T_p$-matching is of the form $\hat{T}_p \bullet AX$, i.e.

$$\mathcal{T}_p = \hat{T}_p \times (C^2 + A).$$

Let $\rho$ be an irreducible shadow with genus $g$ and $m$ arcs and let $\hat{T}_p^\rho$ denote the set of all $\hat{T}_p$ matchings, $\hat{s}$, whose maximal arcs form $\rho$. $\hat{s}$ can be obtained inductively by

- Nest exactly one $T_{p-1}$-matching, $x$, into $\rho$ via the $\bullet$-product, if $\rho$ is a $A$-shadow: $g(x_1) = g(x) + g(\rho)$ and $g(x_1) = g(x) + g(\rho) + 1$, if $\rho$ is a $B$-shadow;

- Inflate each $\rho$-arc into a sequence of induced arcs, $\nu \in \mathcal{M}$, then we have $g(x_2) = g(x_1) + g(\nu)$;

- Inflate each exterior arc in $x_2$ into a stack. There is no change in topological genus here, $g(x_3) = g(x_2)$;

- Insert some $C$-matchings, $c_1, \ldots, c_k$ into the $(2m - 2)$ $\sigma$-intervals of $\rho$, then $g(\hat{s}) = g(x_3) + \sum_{j} g(c_j)$.

Accordingly

$$\hat{T}_p^{\rho A} = T_{p-1} \times (\text{SEQ}(\mathcal{U}) \times \text{SEQ}(\text{SEQ}(\mathcal{U}) \times (C^2 - 1)))^m \times C^{2m-2} \times V^g, \quad (27)$$

and

$$\hat{T}_p^{\rho B} = T_{p-1} \times (\text{SEQ}(\mathcal{U}) \times \text{SEQ}(\text{SEQ}(\mathcal{U}) \times (C^2 - 1)))^m \times C^{2m-2} \times V^{g+1}. \quad (28)$$
Since the above constructions only depend on the number of arcs of \( q \), and 
\( \mathcal{T}_p = \tilde{\mathcal{T}}_p \times (C^2 + A) \), we have

\[
\mathcal{T}_p = \mathcal{T}_{p-1} \times \left( \sum_{g,m} i_{2,A_g}(m) (\text{SEQ}(U) \times \text{SEQ}(\text{SEQ}(U) \times (C^2 - 1)))^m \right) \\
\times C^{2m-2} \times V^g + \sum_{g,m} i_{2,B_g}(m) (\text{SEQ}(U) \times \text{SEQ}(\text{SEQ}(U) \times (C^2 - 1)))^m \\
\times C^{2m-2} \times V^{g+1} \times (C^2 + A).
\]

(29)

This implies

\[
\mathbf{T}_p(u, t) = \mathbf{T}_{p-1}(u, t) \cdot \left[ I_{2,A} \left( \frac{uC(u,t)^2}{1 - uC(u,t)^2}, t \right) + t \cdot I_{2,B} \left( \frac{uC(u,t)^2}{1 - uC(u,t)^2}, t \right) \right] \\
\cdot (A(u, t) + C(u, t)^2) \cdot \frac{1}{C(u, t)^2},
\]

(30)

whence Claim 2.2.

Claim 2.1 and Claim 2.2 allow us to recursively calculate \( \mathbf{T}_p(u, t) \), for
\( p \geq 2 \). However, when calculating \( \mathbf{T}_p(u, t) \), we neglected the genus-decrease
in case of pure \( B \)-shadows. In order to correct this we introduce \( \mathbf{K}_p(u, t) \),
i.e. \( \mathbf{Q}_p(u, t) = \mathbf{T}_p(u, t) + \mathbf{K}_p(u, t) \).

Claim 3.

\[
\mathbf{K}_1(u, t) = \left[ (1 - t) \cdot I_{2,B} \left( \frac{uC(u,t)^2}{1 - uC(u,t)^2}, t \right) \right] \cdot C(u, t)^2,
\]

(31)

\[
\mathbf{K}_p(u, t) = \mathbf{K}_{p-1}(u, t) \cdot \left[ t \cdot I_{2,B} \left( \frac{uC(u,t)^2}{1 - uC(u,t)^2}, t \right) \right].
\]

(32)

To prove the first equation we restrict Claim 1 and Claim 2.1 to the case of
pure \( B \)-shadows. As for the second equation, we restrict Claim 2.2 to pure
\( B \)-shadows and notice that following the proof of Claim 2.2, ignoring the
decrease of genus by one in case of pure \( B \)-shadows, does not affect recursion

25
Therefore Claim 3 follows which allows us obtain $K_p(u, t)$ for all $p \geq 2$. Consequently,

$$Q(u, t) = Q_0(u, t) + Q_1(u, t) + \sum_{p \geq 2} (T_p(u, t) + K_p(u, t)),$$  \hspace{1cm} (33)

where $Q_0(u, t)$ and $Q_1(u, t)$ follows from Claim 0 and Claim 1, $T_p(u, t)$ via the Claims 2.1 and 2.2 and $K_p(u, t)$ via Claim 3.

Setting $I_{2,A} = I_{2,A} \left( \frac{uC(u,t)}{1-uC(u,t)^2}, t \right)$ and $I_{2,B} = I_{2,B} \left( \frac{uC(u,t)}{1-uC(u,t)^2}, t \right)$, we obtain

$$Q(u, t) = \frac{C(u, t)^2 (I_{2,A} + I_{2,B} - tI_{2,B}^2 - I_{2,A}I_{2,B} + uC(u, t)^2(1 - I_{2,B}))}{(1 - tI_{2,B})(1 - uC(u, t)^2 - I_{2,A} - tI_{2,B})},$$  \hspace{1cm} (34)

and the proof of the theorem is complete.

Corollary 3.2. $I_{2,A_g}(y)$ and $I_{2,B_g}(y)$ can be computed as follows:

- $I_{2,A_0}(y) = 0$,
- $I_{2,A_g+1}(y)$ can be computed recursively via $I_{g+1}(y)$, $I_{2,A_i}(y)$, $I_{2,B_i}(y)$, $Q_i(y)$ and $C_i(y)$, where $i \leq g$,
- 
  $I_{2,B_g}(y) = 2(y^2 + y) \frac{dI_{g+1}(y)}{dy} - I_{g+1}(y) - I_{2,A_{g+1}}(y).$  \hspace{1cm} (35)

Proof. We prove the Corollary (3.2) in Section (6).

In light of Corollary (3.2), it suffices to compute $C_g(y)$, $I_g(y)$ and $Q_g(y)$.

As for $C_g(y)$, suppose first $g = 0$. Then $C_0(y)$ is the generating function of the Catalan numbers, i.e. $C_0(y) = \frac{1 - \sqrt{1 - 4y}}{2y}$. For $g \geq 1$, $C_g(y) = \sum c_g(n)y^n$

26
has been computed in (Harer and Zagier, 1986) and (Penner, 1988). The key recursion discovered by (Harer and Zagier, 1986) reads

**Lemma 3.3.** (Harer and Zagier, 1986) The $c_g(n)$ satisfy the recursion

$$(n + 1)c_g(n) = 2(2n - 1)c_g(n - 1) + (2n - 1)(n - 1)(2n - 3)c_{g-1}(n - 2), \quad (36)$$

where $c_g(n) = 0$ for $2g > n$.

The polynomials $I_g(y)$ have already been computed in (Han et al., 2012), the idea there is to construct an analogue of Corollary (3.2):

**Lemma 3.4.** For $g \geq 1$, $I_g(y)$ satisfies the following recursion

$$I_g(y) = C_g(\theta(y)) - \theta(y) \sum_{i=0}^{g} C_i(\theta(y)) C_{g-i}(\theta(y))$$

$$- \sum_{j=1}^{g-1} [t^{g-j}] I_j \left( \frac{\theta(y)(\sum_{k=0}^{g-i} C_k(\theta(y))t^k)^2}{1 - \theta(y)(\sum_{k=0}^{g-i} C_k(\theta(y))t^k)^2} \right), \quad (37)$$

where $\theta(y) = \frac{y(y+1)}{(2y+1)^2}$.

In particular,

$$I_1(y) = y^2(1 + y)^2,$$

$$I_2(y) = y^4(1 + y)^4(17 + 92y + 96y^2),$$

$$I_3(y) = y^6(1 + y)^6(1259 + 15928y + 61850y^2 + 92736y^3 + 47040y^4).$$

$Q_g(y)$, the generating function of 2-backbone matchings of genus $g$ has been computed in (Han and Reidys, 2013). Here the authors established a bijection between unicellular maps (Chapuy, 2010) and bicellular maps. Their bijection has the following enumerative corollary
Corollary 3.5. The generating function $Q_g(y)$ and $C_g(y)$ satisfy the following functional equation

$$
\sum_{g_1=0}^{g+1} C_{g_1}(y)C_{g+1-g_1}(y) + Q_g(y) = C_{g+1}(y)/y, \quad (38)
$$

which is equivalent to the coefficient equation

$$
\sum_{g_1=0}^{g+1} \sum_{i \geq 0} c_{g_1}(i)c_{g+1-g_1}(n-i) + q_g(n) = c_{g+1}(n+1). \quad (39)
$$

Accordingly we derive

$I_{2,A_0}(y) = 0,$

$I_{2,A_1}(y) = y^3(11 + 18y + 8y^2),$

$I_{2,A_2}(y) = y^5(y + 1)(928 + 5378y + 12515y^2 + 14520y^3 + 8376y^4 + 1920y^5),$

$I_{2,A_3}(y) = y^7(y + 1)^2(162158 + 1835979y + 8891051y^2 + 24076143y^3 + 39943686y^4 + 41655548y^5 + 26715416y^6 + 9649920y^7 + 1505280y^8),$

$I_{2,B_0}(y) = y^2(3 + 3y + y^2),$

$I_{2,B_1}(y) = y^4(y + 1)(119 + 529y + 991y^2 + 960y^3 + 476y^4 + 96y^5),$

$I_{2,B_2}(y) = y^6(y + 1)^2(13849 + 130518y + 538113y^2 + 1263849y^3 + 1847182y^4 + 1719618y^5 + 995738y^6 + 327936y^7 + 47040y^8).$
4 Two back-bones $\gamma$-matchings

According to Corollary (3.2), we can recursively compute $I_{2,A_g}(u)$ and $I_{2,B_g}(u)$. Let

$$I_{2,\gamma_A}(u, t) = \sum_{g \leq \gamma} I_{2,A_g}(u)t^g,$$

$$I_{2,\gamma_B}(u, t) = \sum_{g \leq \gamma} I_{2,B_g}(u)t^g.$$  

(40)  

(41)

Particularly, for $\gamma = 0$ and 1, we have

$$I_{2,0_A}(u, t) = 0,$$

$$I_{2,0_B}(u, t) = (3u^2 + 3u^3 + u^4)t^0 = 3u^2 + 3u^3 + u^4,$$

$$I_{2,1_A}(u, t) = (7u^3 + 6u^4)t,$$

$$I_{2,1_B}(u, t) = 3u^2 + 3u^3 + u^4 + (4u^3 + 131u^4 + 656u^5 + 1520u^6 + 1951u^7 + 1436u^8 + 572u^9 + 96u^{10})t.$$

Let furthermore $h_{\gamma}(g, n)$ denote the number of $\gamma$-matchings of genus $g$ with $n$ arcs. Then

$$H_{\gamma}(u) = \sum_{g \leq \gamma} \sum_{n} h_{\gamma}(g, n)u^n,$$

$$H_{\gamma}(u, t) = \sum_{g \leq \gamma} \sum_{n} h_{\gamma}(g, n)u^n t^g.$$  

(42)

$H_{\gamma}(u, t)$ has already been given in (Li and Reidys, 2012).

Furthermore, let $q_{\gamma}(g, n)$ denote the number of $\gamma$-interaction matchings of genus $g$ with $n$ arcs and

$$Q_{\gamma}(u) = \sum_{g \leq \gamma} \sum_{n} q_{\gamma}(g, n)u^n,$$

$$Q_{\gamma}(u, t) = \sum_{g \leq \gamma} \sum_{n} q_{\gamma}(g, n)u^n t^g.$$  

(43)

We next compute the generating function $\gamma$-matchings over two backbones, $Q_{\gamma}(u, t)$. We can see that $Q_{\gamma}(u, t)$ and $Q(u, t)$, discussed in Section [3],
differ only in terms of the range of the summation index of \( g \). As a result, the proof of Theorem (3.1) can be duplicated and we derive

**Corollary 4.1.** The bivariate generating function of \( \gamma \)-matchings over two backbones: \( Q_\gamma(u, t) \), satisfies

\[
Q_\gamma(u, t) = \frac{H_\gamma(u, t)^2 \left( I_{2, \gamma_A} + I_{2, \gamma_B} - tI_{2, \gamma_B}^2 - I_{2, \gamma_A}I_{2, \gamma_B} + uH_\gamma(u, t)^2(1 - I_{2, \gamma_B}) \right)}{(1 - tI_{2, \gamma_B})(1 - uH_\gamma(u, t)^2 - I_{2, \gamma_A} - tI_{2, \gamma_B})},
\]

(44)

where \( I_{2, \gamma_A} = I_{2, \gamma_A} \left( \frac{uH_\gamma(u, t)^2}{1 - uH_\gamma(u, t)^2}, t \right) \) and \( I_{2, \gamma_B} = I_{2, \gamma_B} \left( \frac{uH_\gamma(u, t)^2}{1 - uH_\gamma(u, t)^2}, t \right) \).

## 5 Discussion

In this section we address \( \gamma \)-interaction structures and their genus distribution. The passage from \( \gamma \)-matchings to \( \gamma \)-interaction structures employs the notion of shapes. A matching \( X \) is a *shape* if each stack in \( X \) is of length exactly one. Given an arbitrary matching \( s \), its shape is obtained by collapsing each stack to a single arc and then removing any isolated vertices from the thus obtained diagram.

Let \( S_\gamma \) denote the set of shapes that are \( Q_\gamma \)-matchings and let \( Q_\gamma(n, m) \) denote the combinatorial class of \( Q_\gamma \)-matchings over \( 2n \) vertices with \( m \) interior arcs of length 1 (1-arcs). Note that any 1-arc is by definition an interior arc. Furthermore, let \( S_\gamma(n, m, g) \) denote the class of all \( S_\gamma \)-shapes over \( 2n \) vertices with \( m \) 1-arcs of genus \( g \) with generating function \( S_\gamma(u, e, t) \). Since collapsing stacks, adding or deleting 1-arcs do not affect genus, we can enrich the functional equation given in Lemma 6.1 of [Qin and Reidys, 2012].
by means of a genus filtration:

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

(45)

It is straightforward to obtain a \( \tau \)-canonical \( \gamma \)-interaction structure from a shape by inserting isolated vertices and inflating arcs to stacks. All of these steps will not change the topological genus. Thus we can extend \( Q_{\tau, \gamma}(z) \) of [Qin and Reidys, 2012] to a bivariate generating function. By symbolic methods, we eventually derive

**Theorem 5.1.** Suppose \( \gamma \geq 0 \) and \( \tau \geq 1 \) and let \( u_\tau(z) = \frac{(z^2)^{\gamma-1}}{z^{2\gamma} - z + 1} \). Then the generating function of \( \tau \)-canonical \( \gamma \) structures over two backbones is given by

\[ Q_{\tau, \gamma}(z, t) = \frac{1}{(u_\tau(z)z^2 - z + 1)^2} Q_{\gamma} \left( \frac{u_\tau(z)z^2}{(u_\tau(z)z^2 - z + 1)^2}, t \right). \]  

(46)

Let us secondly discuss the genus distribution of \( \gamma \)-interaction structures. For this purpose, we study the random variable \( X_{n, \tau, \gamma} \) having the distribution

\[ P(X_{n, \tau, \gamma} = g) = \frac{Q_{\tau, \gamma}(n, g)}{Q_{\tau, \gamma}(n)}, \]  

(47)

where \( g = 0, 1, \ldots, \lfloor \frac{n-1}{2} \rfloor \).

In case of \( \gamma = 0, 1 \), \( Q_{\gamma, \tau}(z, t) \) has the unique dominant singularity \( \theta(t) \), where we compute a local, singular representation of the form

\[ Q_{\gamma, \tau}(z, t) = g(z, t) + h(z, t) \left( 1 - \frac{z}{\theta(t)} \right)^\alpha \]  

(48)

for some real \( \alpha \in \mathbb{R} - \mathbb{N} \) and functions \( g(z, t), h(z, t) \neq 0 \) and \( \theta(t) \neq 0 \) that are analytic at \( z = z_0 > 0 \) and \( t = 1 \). If \( t \) is sufficiently close to 1, there exists an analytic continuation of \( Q_{\gamma, \tau}(z, t) \) to the region \( |z| < |\theta(t)| + \delta, |\arg(z - \theta(t))| > \epsilon \) for some \( \delta > 0 \) and \( \epsilon > 0 \).
The two parameter version of the transfer lemma of Flajolet and Sedgewick (2009) in combination with the Quasi Power Theorem (Hwang, 1998) implies Theorem 5.2.

For \( \gamma = 0,1 \) and \( 1 \leq \tau \leq 10 \), there exists a pair \( (\mu_{\tau,\gamma}, \sigma_{\tau,\gamma}) \) such that the normalized random variable

\[
Y_{n,\tau,\gamma} = \frac{X_{n,\tau,\gamma} - \mu_{\tau,\gamma} n}{\sqrt{n} \sigma_{\tau,\gamma}},
\]

converges in distribution to a Gaussian variable with \( \mu_{\tau,\gamma} \) and \( \sigma_{\tau,\gamma}^2 \) are given by

\[
\mu_{\tau,\gamma} = -\frac{\theta'(1)}{\theta(1)} \quad \text{and} \quad \sigma_{\tau,\gamma}^2 = -\frac{\theta''(1)}{\theta(1)} - \frac{\theta'(1)}{\theta(1)} + \left( \frac{\theta'(1)}{\theta(1)} \right)^2.
\]

Furthermore there exist positive constants \( c_1, c_2, c_3 \) such that

\[
P\{||X_n - EX_n|| \geq \epsilon \sqrt{n} \} \leq c_1 e^{-c_2 \epsilon^2},
\]

uniformly for \( \epsilon \leq c_3 \sqrt{n} \).

In Table 1, we present the values of the pairs \( (\mu_{\tau,\gamma}, \sigma_{\tau,\gamma}) \) for \( \gamma = 0,1 \).

6 Appendix

Proof of Corollary (3.2).

Proof. Claim 1.

\[
\begin{align*}
& \left( I_{2,A_{g}}(y) + \sum_{j=0}^{g-1} [t^{g-j}] I_{2,A_{j}}(\omega(\theta(y), t)) \right) \left[ C_0^2(\theta(y)) (1 - I_{2,B_0}(y)) + Q_0(\theta(y)) \right] \\
+ & \left( I_{2,B_g}(y) + \sum_{j=0}^{g-1} [t^{g-j}] I_{2,B_{j}}(\omega(\theta(y), t)) \right) \left[ C_0^2(\theta(y)) - \theta(y) C_0^4(\theta(y)) \right] \\
= & M(\theta(y)).
\end{align*}
\]
where $\omega(\theta(y), t) = \frac{\theta(y)C^2(\theta(y), t)}{1 - \theta(y)C^2(\theta(y), t)}$, $\theta(y) = \frac{y(y+1)}{(2y+1)^2}$ and $M(\theta(y))$ is a polynomial in the variable $y$.

To prove Claim 1, we consider equation (10) of Theorem (3.1), multiply the denominator of the right hand side on both sides of it and then compute

$$
[t^g]Q(u, t) + u[t^{g-1}]C^2(u, t)I_{2,B}Q(u, t) + [t^{g-1}]J_{2,A}I_{2,B}Q(u, t)
$$

$$
+ [t^{g-2}]J_{2,B}Q(u, t) - u[t^g]C^2(u, t)Q(u, t) - [t^g]I_{2,A}Q(u, t) - 2[t^{g-1}]I_{2,B}Q(u, t)
$$

$$
= [t^g](I_{2,A} + I_{2,B})C^2(u, t) + u[t^g]C^4(u, t)
$$

$$
- [t^{g-1}]J_{2,B}C^2(u, t) - [t^g]J_{2,A}I_{2,B}C^2(u, t) - u[t^g]I_{2,B}C^4(u, t).
$$

Notice that $[t^g]Q(u, t) = Q_g(u)$, and

$$
[t^g]J_{2,A} \left( \frac{uC^2(u, t)}{1 - uC^2(u, t)}, t \right) = \sum_{j=0}^{g} [t^{g-j}]J_{2,A_j} \left( \frac{uC^2(u, t)}{1 - uC^2(u, t)} \right),
$$

$$
[t^g]J_{2,B} \left( \frac{uC^2(u, t)}{1 - uC^2(u, t)}, t \right) = \sum_{j=0}^{g} [t^{g-j}]J_{2,B_j} \left( \frac{uC^2(u, t)}{1 - uC^2(u, t)} \right).
$$

Let $\omega(u, t) = \frac{uC^2(u, t)}{1 - uC^2(u, t)}$, by the above we have now a recursion for $I_{2,A_g}(u)$ and $I_{2,B_g}(u)$. In view of $I_{2,A_0}(u) = 0$, we have
\[ [t^g]I_{2,A}(\omega(u, t), t) \left[ C_0(u)^2 - I_{2,B_0} \left( \frac{u C_0(u)^2}{1 - u C_0(u)^2} \right) + Q_0(u) \right] \]

\[ + [t^g]I_{2,B}(\omega(u, t), t) \left[ C_0(u)^2 - u C_0(u)^4 \right] \]

\[ = Q_g(u) - u[t^g]C(u, t)^2Q(u, t) - 2[t^{g-1}]I_{2,B}(\omega(u, t), t)Q(u, t) \]

\[ + u[t^{g-1}]I_{2,B}(\omega(u, t), t)C(u, t)^2Q(u, t) + [t^{g-2}]I_{2,B}(\omega(u, t), t)^2Q(u, t) \]

\[ - \sum_{j=0}^{g-1} [t^j]I_{2,A}(\omega(u, t), t)[t^{g-j}]C(u, t)^2 - \sum_{j=0}^{g-1} [t^j]I_{2,B}(\omega(u, t), t)[t^{g-j}]C(u, t)^2 \]

\[ + \sum_{g_1 + g_2 + g_3 = g \atop g_1 \leq g-1, g_2 \leq g-1} [t^{g_1}]I_{2,A}(\omega(u, t), t)[t^{g_2}]I_{2,B}(\omega(u, t), t)[t^{g_3}]C(u, t)^2 \]

\[ + u \sum_{j=0}^{g-1} [t^j]I_{2,B}(\omega(u, t), t)[t^{g-j}]C(u, t)^4 + [t^{g-1}]I_{2,B}(\omega(u, t), t)I_{2,A}(\omega(u, t), t) \]

\[ \cdot Q(u, t) + [t^{g-1}]I_{2,B}(\omega(u, t), t)^2C(u, t)^2 - u[t^g]C(u, t)^4 \]

\[ - \sum_{j=0}^{g-1} [t^j]I_{2,A}(\omega(u, t), t)[t^{g-j}]Q(u, t). \]

We denote the right side of the above equation by \( M(u) \), and set \( y = \frac{z C_0^2(u)}{1 - u C_0(u)^2} \). Then \( u = \theta(y) = \frac{y(y+1)}{(2y+1)^2} \) and we derive

\[
\left( I_{2,A}(y) + \sum_{j=0}^{g-1} [t^{g-j}]I_{2,A_j}(\omega(\theta(y), t)) \right) \left[ C_0^2(\theta(y))(1 - I_{2,B_0}(y)) + Q_0(\theta(y)) \right] 
\]

\[
+ \left( I_{2,B}(y) + \sum_{j=0}^{g-1} [t^{g-j}]I_{2,B_j}(\omega(\theta(y), t)) \right) \left[ C_0^2(\theta(y)) - \theta(y) C_0^4(\theta(y)) \right] 
\]

\[ = M(\theta(y)), \quad (53) \]

as claimed. Claim 1 allows us to compute \( I_{2,A_{g+1}}(y) \) via \( I_{g+1}(y), I_{2,A}(y), I_{2,B}(y), Q_i(y) \) and \( C_i(y) \), where \( i \leq g \), as stipulated in Corollary (3.2).
Claim 2.

\[ I_{2,B_g}(y) + I_{2,A_{g+1}}(y) = 2(y^2 + y) \frac{dI_{g+1}(y)}{dy} - I_{g+1}(y). \]  \hspace{1cm} (54)

To prove Claim 2, it suffices to show

\[ i_{2,A_g}(m) + i_{2,B_g-1}(m) = (2m - 1)i_g(m) + 2(m - 1)i_g(m - 1), \]  \hspace{1cm} (55)

where \( i_g(m) \) is the number of irreducible shadows of genus \( g \) having \( m \) arcs over 1 backbone. Furthermore, \( i_{2,A_g}(m) \) and \( i_{2,B_g-1}(m) \) denote the number of irreducible \( A \)- and \( B \)-shadows.

Close inspection of Lemma (2.1) shows that it induces a bijection of irreducible shadows, where we define a \( d \)-shadow to be irreducible if it is induced by an irreducible shadow (by inflating an arc into a stack of size two). That is any irreducible 2-backbone shadow can be obtained by cutting either an irreducible 1-backbone shadow or an irreducible \( d \)-shadow. This however implies recursion (55). To see this, we observe that an irreducible 1-shadow with \( m \) arcs has \((2m - 1)\) cut-points and any \( s \in D_{g,m} \) has two cut-points, the number of irreducible \( d \)-shadows with \( m \) arcs being \((m - 1)i_g(m - 1)\).

It thus remains to translate the recursion to an equation of generating functions:

\[ I_{2,B_g}(y) + I_{2,A_{g+1}}(y) = 2(y^2 + y) \frac{dI_{g+1}(y)}{dy} - I_{g+1}(y), \]  \hspace{1cm} (56)

as claimed. We computed \( I_{2,A_{g+1}}(y) \) in Claim 1 and substitution yields

\[ I_{2,B_g}(y) = 2(y^2 + y) \frac{dI_{g+1}(y)}{dy} - I_{g+1}(y) - I_{2,A_{g+1}}(y). \]  \hspace{1cm} (57)

There are no irreducible \( A \)-shadows of genus 0, whence \( I_{2,A_0}(y) = 0 \). \( \Box \)
Acknowledgements

We want to thank Fenix Wen Da Huang and Thomas Jia Xian Li for discussions.

Author Disclosure Statement

No competing financial interests exist.

References

C. Alkan, E. Karakoc, J. H. Nadeau, S. C. Sahinalp, and K. Z. Zhang. 2006. RNA-RNA interaction prediction and antisense RNA target search. *J. Comp. Biol.*, 13:267–282.

J. E. Andersen, F. W. D. Huang, R. C. Penner, and C. M. Reidys. 2012a. Topology of RNA-RNA interaction structures. *J. Comp. Biol.*, 19(7):928–943.

J. E. Andersen, R. C. Penner, C. M. Reidys, and M. S. Waterman. 2012b. Topological classification and enumeration of RNA structures by genus. *J. Math. Bio*. preprint.

S. Bernhart, H. Tafer, U. Mückstein, C. Flamm, P. F. Stadler, and I. L. Hofacker. 2006. Partition function and base pairing probabilities of RNA heterodimers. *Alg. Mol. Biol.*. 1:3.
M. Bon, G. Vernizzi, H. Orland, and A. Zee. 2008. Topological classification of RNA structures. *J. Mol. Biol.*, 379:900–911.

A. Busch, A. S. Richter, and R. Backofen. 2008. Efficient prediction of bacterial sRNA targets incorporating target site accessibility and seed regions. *Bioinformatics*, 24:2849–2856.

G. Chapuy. 2010. The structure of unicellular maps, and a connection between maps of positive genus and planar labelled trees. *Probability Theory and Related Fields*, 147(3):415–447.

P. Flajolet and R. Sedgewick. 2009. *Analytic Combinatorics*. Cambridge University Press New York.

H. S. W. Han and C. M. Reidys. 2013. A bijection between unicellular and bicellular map.

H. S. W. Han, T.J.X.Li, and C. M. Reidys. 2012. Combinatorics of $\gamma$-structures. *E. J. Combin*. submitted.

J. Harer and D. Zagier. 1986. The euler characteristic of the moduli space of curves. *Invent.Math.*, 85:457–486.

I. L. Hofacker, W. Fontana, P. F. Stadler, L. S. Bonhoeffer, M. Tacker, and P. Schuster. 1994. Fast folding and comparison of RNA secondary structures. *Monatsh. Chem.*, 125:167–188.

F. W. D. Huang, J. Qin, P. F. Stadler, and C. M. Reidys. 2009. Partition function and base pairing probabilities for RNA-RNA interaction prediction. *Bioinformatics*, 25(20):2646–2654.
F. W. D. Huang, J. Qin, C. M. Reidys, and P. F. Stadler. 2010. Target prediction and a statistical sampling algorithm for RNA-RNA interaction. *Bioinformatics*, 26:175–181.

H. K. Hwang. 1998. On convergence rates in the central limit theorems for combinatorial structures. *European J. Combin.*, 19:329–343. MR 99c:60014.

A. M. Kiss, B. E. Jady, E. Bertrand, and T. Kiss. 2004. Human box H/ACA pseudouridylation guide RNA machinery. *Mol. Cell. Biol.*, 24:5797–5807.

T. J. X. Li and C. M. Reidys. 2012. The genus filtration of $\gamma$-structures. *Math. Biosc.* in revision.

H. Ly, L. Xu, M. A. Rivera, T. G. Parslow, and E. H. Blackburn. 2003. A role for a novel ‘trans-pseudoknot’ RNA-RNA interaction in the functional dimerization of human telomerase. *Genes & Dev.*, 17:1078–1083.

W. S. Massey. 1967. *Algebraic Topology: An Introduction*. Springer-Verlag, New York.

U. Mückstein, H. Tafer, J. Hackermüller, S. H. Bernhard, P. F. Stadler, and I. L. Hofacker. 2006. Thermodynamics of RNA-RNA binding. *Bioinformatics*, 22:1177–1182.

U. Mückstein, H. Tafer, S. H. Bernhard, M. Hernandez-Rosales, J. Vogel, P. F. Stadler, and I. L. Hofacker. 2008. Translational control by RNA-RNA interaction: Improved computation of RNA-RNA binding thermodynamics. *Comm. Comp. Inf. Sci.*, 13:114–127, Berlin, Springer. In Mourad Elloumi, Josef Küng, Michal Linial, Robert F. Murphy, Kristan Schneider,
and Cristian Toma Toma, editors, BioInformatics Research and Development — BIRD 2008.

J. Ofengand and A. Bakin. 1997. Mapping to nucleotide resolution of pseudouridine residues in large subunit ribosomal RNAs from representative eukaryotes, prokaryotes, archaebacteria, mitochondria and chloroplasts. J. Mol. Biol., 266:246–268.

H. Orland and A. Zee. 2002. RNA folding and large $n$ matrix theory. Nuclear Physics B, 620:456–476.

R. C. Penner. 2004. Cell decomposition and compactification of Riemann’s moduli space in decorated Teichmüller theory. In Nils Tongring and R. C. Penner, editors, Woods Hole Mathematics-perspectives in math and physics, pages 263–301. World Scientific, Singapore, arXiv:math. GT/0306190.

R. C. Penner. 1988. Perturbative series and the moduli space of Riemann surfaces. B. J. Differential Geom, 27(1).

R. C. Penner. 2011. Decorated teichmüller theory. In European Mathematical Society, Zürich.

R. C. Penner and M. S. Waterman. 1993. Spaces of RNA secondary structures. Adv. Math., 101:31–49.

R. C. Penner, M. Knudsen, C. Wiuf, and J. E. Andersen. 2010. Fatgraph models of proteins. Comm. Pure Appl. Math., 63:1249–1297.
D. D. Pervouchine. 2004. IRIS: Intermolecular RNA interaction search. Proc. Genome Informatics, 15:92–101.

J. Qin and C. M. Reidys. 2012. On topological RNA interaction structures. J. Comp. Biol. accepted.

C. M. Reidys, R. R. Wang, and A. Y. Y. Zhao. 2010. Modular, k-noncrossing diagrams. E.J. Combin. (17), 1, R76.

C. M. Reidys, F. W. D. Huang, J. E. Andersen, R. C. Penner, P. F. Stadler, and M. E. Nebel. 2011. Topology and prediction of RNA pseudoknots. Bioinformatics, 27:1076–1085.

E. Rivas and S. R. Eddy. 1999. A dynamic programming algorithms for RNA structure prediction including pseudoknots. J. Mol. Biol., 285:2053–2068.

G. Vernizzi and H. Orland. 2005. Large-\(N\) random matrices for RNA folding. Acta. Phys. Polon., 36:2821–2827.
| τ  | $\mu_{\tau,\gamma}$ | $\sigma^2_{\tau,\gamma}$ | $\mu_{\tau,\gamma}$ | $\sigma^2_{\tau,\gamma}$ | $\mu_{\tau,\gamma}$ | $\sigma^2_{\tau,\gamma}$ |
|-----|----------------------|-----------------------------|----------------------|-----------------------------|----------------------|-----------------------------|
| $\gamma = 0$ | 0.065198 | 0.087702 | 0.029719 | 0.010128 | 0.019179 | 0.006550 |
| $\gamma = 1$ | 0.091240 | 0.021067 | 0.041235 | 0.009358 | 0.026632 | 0.006043 |
| $\gamma = 0$ | 0.014168 | 0.004855 | 0.011245 | 0.003864 | 0.009331 | 0.003214 |
| $\gamma = 1$ | 0.019706 | 0.004481 | 0.015666 | 0.003571 | 0.013017 | 0.002974 |

Table 1: Genus distribution: the central limit theorem for topological genus in $\gamma$-interaction structures, for genus equals 0 and 1, and $1 \leq \tau \leq 6$, we computed $\mu$ and $\sigma^2$ as in the table.