On the uniform generation of modular diagrams

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Abstract

In this paper we present an algorithm that generates $k$-noncrossing, $\sigma$-modular diagrams with uniform probability. A diagram is a labeled graph of degree $\leq 1$ over $n$ vertices drawn in a horizontal line with arcs $(i,j)$ in the upper half-plane. A $k$-crossing in a diagram is a set of $k$ distinct arcs $(i_1,j_1),(i_2,j_2),\ldots,(i_k,j_k)$ with the property $i_1 < i_2 < \ldots < i_k < j_1 < j_2 < \ldots < j_k$. A diagram without any $k$-crossings is called a $k$-noncrossing diagram and a stack of length $\sigma$ is a maximal sequence $((i,j),(i+1,j-1),\ldots,(i+(\sigma-1),j-(\sigma-1)))$. A diagram is $\sigma$-modular if any arc is contained in a stack of length at least $\sigma$. Our algorithm generates after $O(n^k)$ preprocessing time, $k$-noncrossing, $\sigma$-modular diagrams in $O(n)$ time and space complexity.

Keywords: $k$-noncrossing diagram, uniform generation, RSK-algorithm

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1. Introduction

A ribonucleic acid (RNA) molecule is the helical configuration of a primary structure of nucleotides, A, G, U and C, together with Watson-Crick (A-U, G-C) and (U-G) base pairs (arcs). It is well-known that RNA structures exhibit cross-serial nucleotide interactions, called pseudoknots. First recognized in the turnip yellow mosaic virus in [7], they are now known to be widely conserved in functional RNA molecules.

Modular k-noncrossing diagrams represent a model of RNA pseudoknot structures [4, 5], that is RNA structures exhibiting cross-serial base pairings. The particular case of modular noncrossing diagrams, i.e. RNA secondary structures have been extensively studied [3, 6, 8, 9].

A diagram is a labeled graph over the vertex set \([n] = \{1, \ldots, n\}\) with vertex degrees not greater than one. The standard representation of a diagram is derived by drawing its vertices in a horizontal line and its arcs \((i, j)\) in the upper half-plane. A \(k\)-crossing is a set of \(k\) distinct arcs \((i_1, j_1), (i_2, j_2), \ldots, (i_k, j_k)\) with the property

\[i_1 < i_2 < \ldots < i_k < j_1 < j_2 < \ldots < j_k.\]

A diagram without any \(k\)-crossings is called a \(k\)-noncrossing diagram. Furthermore, a stack of length \(\sigma\) is a maximal sequence of “parallel” arcs,

\[((i, j), (i + 1, j − 1), \ldots, (i + (\sigma − 1), j − (\sigma − 1)))\]

and is also referred to as a \(\sigma\)-stack. A \(k\)-noncrossing diagram having only stacks of lengths one is called a core.

Biophysical structures do not exhibit any isolated bonds. That is, any arc in their diagram representation is contained in a stack of length at least two. We call a
Figure 1. \(k\)-noncrossing diagrams: a 4-noncrossing diagram (left) and a 2-noncrossing diagram (right). The arcs \((2, 6), (4, 8)\) and \((5, 11)\) form a 3-crossing in the left diagram.

diagram, whose arcs are contained in stacks of lengths at least \(\sigma\), \(\sigma\)-modular. Modular, \(k\)-noncrossing diagrams are likely candidates for natural molecular structures. Sequence lengths of interest for such structures range from 75–300 nucleotides.

The main result of this paper is an algorithm that generates \(k\)-noncrossing, \(\sigma\)-modular diagrams with uniform probability. Our construction is motivated by the ideas of [2], where a combinatorial algorithm has been presented that uniformly generates \(k\)-noncrossing diagrams in \(O(n^k)\) time complexity. To be precise, we generate \(k\)-noncrossing modular diagrams “locally” having a success rate that depends on specific parameters, see Fig. 2.

The paper is organized in two sections. In Section 2 we lay the foundations for our main result by generating core diagrams with uniform probability. In Section 3 we introduce weighted cores and subsequently prove the main theorem.

2. Core diagrams

A shape \(\lambda\) is a set of squares arranged in left-justified rows with weakly decreasing number of boxes in each row. A Young tableau is a filling in squares in the shape with numbers, which is weakly increasing in each row and strictly increasing in each
Figure 2. Uniformity and success-rate of Algorithm 2. We run Algorithm 2 for $5 \times 10^6$ times attempting to generate 3-noncrossing 2-modular diagrams over 20 vertices. 4,354,410 of these executions generate a modular diagram. In (a) we display the frequency distribution of multiplicities (dots) and the Binomial distribution (curve). In (b) we display the success rate of Algorithm 2 as a function of $n$ for the following classes of modular diagrams: $k = 3, \sigma = 2$ ([1]), $k = 4, \sigma = 2$ ([2]) and $k = 5, \sigma = 2$ ([3]).

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\[ \emptyset = \lambda^0, \lambda^1, \ldots, \lambda^n, \]

such that $\lambda^i$ differ from $\lambda^{i-1}$ by at most one square. See Fig. 3 (a).

According to [1] we have a bijection between $k$-noncrossing diagrams and a *-tableaux of $\emptyset$ having at most $(k - 1)$ rows. Let us make the bijection explicit: reading the *-tableaux having $n$ steps from left to right we do the following: if $\lambda^i \setminus \lambda^{i-1} = +\square$, we insert $i$ in the new square. Otherwise if $\lambda^i \setminus \lambda^{i-1} = -\square$, we extract the unique entry $j$ via inverse RSK algorithm [1, 2] and form an arc $(j, i)$. By inverse RSK algorithm we mean the following: given a Young tableau $Y^i$ of shape $\lambda^i$ and a shape $\lambda^{i+1}$ such that $\lambda^{i+1} \setminus \lambda^i = -\square$, there exists a unique entry $j$ of
and a Young tableau $Y^{i+1}$ of shape $\lambda^{i+1}$ such that RSK-insertion of $j$ into $Y^{i+1}$ recovers $Y^i$. Finally, in case of $\lambda^i \setminus \lambda^{i-1} = \emptyset$ we do nothing, see Fig. 3. Given a $k$-noncrossing diagram, we read the vertices from right to left and initialize $\lambda^n = \emptyset$. If $i$ is a terminal of an arc, $(j, i)$, we obtain $\lambda^{i-1}$ by inserting $j$ into $\lambda^i$ via RSK insertion. If $i$ is an isolated vertex we do nothing, and remove the square contain $i$ when it is an origin of an arc, see Fig. 3.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure3.png}
\caption{From $*$-tableaux to diagrams and back. Reading (a) from left to right, we insert $i$ into the new square in case of $\lambda^i \setminus \lambda^{i-1}$ being a $-\square$-step and extract the square via inverse RSK if $\lambda^i \setminus \lambda^{i-1}$ is a $-\square$-step. The extraction leads to an arc. Reading (c) from right to left, $\lambda^{i-1}$ is obtained by RSK insertion of $j$ into $\lambda^i$ if $i$ is the terminal of an arc. We do nothing if $i$ is an isolated vertex and we remove the square with entry $i$ in case of $i$ being an origin of an arc.

Let

$$T_i(\lambda) = \left\{ (\lambda^j)_{0 \leq j \leq i} \mid (\lambda^j)_j \text{ is a } *\text{-tableau having at most } (k-1) \text{ rows and } \lambda^i = \lambda \right\}.$$

Any $\vartheta \in T_i(\lambda)$ induces a unique arc-set $A(\vartheta)$. We set $A_0(\vartheta) = \emptyset$ and do the following...}
• for a $+$□-step, we insert $h$ into the new square,
• for a $∅$-step, we do nothing,
• for a $−$□-step, we extract the unique entry, $j(h)$, of the tableaux $Y^{h-1}$ which, if RSK-inserted into $Y^h$, recovers $Y^{h-1}$ and set $A_h(ϑ) = A_{h-1}(ϑ) ∪ \{(j(h), h)\}$.

Setting $A(ϑ) = A_i(ϑ)$ we obtain an induced arc set $A(ϑ)$, as well as a unique sequence of Young tableaux $Y(ϑ) = \{ Y^0 = ∅, Y^1, \ldots, Y^i \}$, where for $h ≤ i$, $Y^h$ is a Young tableau of shape $λ^h$. These extractions generate a set of arcs $(j(i), i)$, which in turn uniquely determines a $k$-noncrossing diagram.

**Lemma 1.** Suppose $r ≥ 1$ and $ϑ_{p,q,r} ∈ T_i(λ)$ is a $∗$-tableaux such that

$$(p, q), (p + 1, q - 1), \ldots, (p + r, q - r)$$

are stacked pairs of insertion-extraction steps. Let $f(ϑ_{p,q,r}) ∈ T_i(λ)$ be the $∗$-tableaux in which all $r$ insertion-extraction pairs $(p + 1, q - 1), \ldots, (p + r, q - r)$ are replaced by $2r ∅$-steps. Then we have a correspondence between $ϑ_{p,q,r}$ and $f(ϑ_{p,q,r})$.

**Proof.** Let $Y(ϑ_{p,q,r})$ denote its associated sequence of Young tableaux,

$$(2.1) \quad (Y^t)_{0 ≤ t ≤ i} = (Y^0 = ∅, Y^1, \ldots, Y^i).$$

We next construct a new sequence of Young tableaux,

$$(2.2) \quad Y(f(ϑ_{p,q})) = \{ J^0, J^1, \ldots, J^n = Y^i \},$$

from right to left via the following algorithm

• for a $−$□-step of the original $∗$-tableaux, $ϑ_{p,q,r}$, let $j$ be the unique entry extracted from $Y^{t-1}$ which if RSK-inserted into $Y^t$ recovers $Y^{t-1}$. If $t = q, q-1, \ldots, q-r$ we do nothing, otherwise: $J^{t-1}$ is obtained by RSK-insertion of $j$ into $J^t$,
• for a $∅$-step, we do nothing,
• for a $+\Box$-step, if $t = p+1, \ldots, p+r$, we do nothing, otherwise $J^{t-1}$ is obtained by removing the square with entry $t$ from $J^t$.

By construction, $J^0 = \emptyset$ and considering the induced sequence of shapes of the sequence of Young tableaux $J^0, \ldots, J^i$ we obtain a unique $*$-tableau $f(\vartheta_{p,q,r})$. By construction $f(\vartheta_{p,q,r})$ has $\emptyset$-steps at step $p+1, \ldots, p+r$ and steps $q-1, \ldots, q-r$, respectively.

Suppose we are given a $*$-tableaux $\psi_{p,q,r}$ having the insertion-extraction pair $(p,q)$ and $\emptyset$-steps at step $p+1, \ldots, p+r$ and $q-1, \ldots, q-r$, respectively together with its sequence of Young tableaux $(J^t)_{0 \leq t \leq i}$. Then we construct the sequence of Young tableaux $(Y^t)_{0 \leq t \leq i}$ initialized $Y^0 = J^0 = \emptyset$:

• for a $-\Box$-step of the original $*$-tableaux, $\psi_{p,q,r}$, let $j$ be the unique entry extracted from $Y^{t-1}$ which if RSK-inserted into $Y^t$ recovers $Y^{t-1}$. $Y^{t-1}$ is obtained by RSK-insertion of $j$ into $Y^t$,
• for a $\emptyset$-step of $\psi_{p,q,r}$, if $t = q-1, \ldots, q-r$, we add a square and insert $p+1, \ldots, p+r$. If $t = p+1, \ldots, p+r$, we remove the square with the respective entry $p+1, \ldots, p+r$. Otherwise, we do nothing.
• for a $+\Box$-step of $\psi_{p,q,r}$, $Y^{t-1}$ is obtained by removing the square with entry $t$.

It is straightforward to verify that the above algorithm is well-defined and recovers the $*$-tableaux $\vartheta_{p,q,r}$ from $f(\vartheta_{p,q,r})$, whence the lemma. See Fig. 4.

We next consider

$$T^c_i(\lambda) = \{t \in T_i(\lambda) \mid \forall a \in A(t), a \text{ is an isolated arc}\}$$

and set $t^c_i(\lambda) = |T^c_i(\lambda)|$. Given a shape $\lambda^i$, let $\lambda_{j+}^{i-1}$ denote the shape from which $\lambda^i$ is obtained by adding a square in the $j$th row, and $\lambda_{j-}^{i-1}$ denote the shape from
which \( \lambda^i \) is derived by removing a square in the \( j \)th row. Thus tracing back a shape \( \lambda^i \) we observe that it is either derived by

- \( \lambda^{i-1}_{j+} \) (obtained by adding a square in the \( j \)th row),
- \( \lambda^{i-1}_0 \) (doing nothing), or
- \( \lambda^{i-1}_{j-} \) (obtained by removing a square in the \( j \)th row).

**Lemma 2.**

\[
(2.4) \quad t_i^c(\lambda^i) = t_{i-1}^c(\lambda^{i-1}_0) + \sum_{j=1}^{k-1} t_{i-1}^c(\lambda^{i-1}_{j+}) + \sum_{j=1}^{k-1} \sum_{p=0}^{\lfloor \frac{i-1}{2} \rfloor} (-1)^p t_{i-1-2p}^c(\lambda^{i-1-2p}_{j-}).
\]

**Proof.** By construction, \( +\square \)-steps as well as \( \emptyset \)-steps do not induce new arcs. An arc \( \alpha \) is only formed when removing a square and such an arc is potentially stacking. Let

\[
G_{i-1}(\lambda^{i-1}_{j-}) = \{ (\lambda^h)_{0 \leq h \leq i-1} \in T_{i-1}^c(\lambda^{i-1}_{j-}) \mid \lambda^i \setminus \lambda^{i-1} = -\square_j \text{ and } \alpha \text{ is stacking} \}.
\]
Thus, for any \( t \in T^c_{i-1}(\lambda_{j-1}^{i-1}) \setminus G_{i-1}(\lambda_{j-1}^{i-1}) \), the \(*\)-tableaux \((t, -\square_j)\) is contained in \(T^c_i(\lambda^i)\). We accordingly arrive at

\[
T^c_i(\lambda) = T^c_{i-1}(\lambda_{0}^{i-1}) \cup \left( \bigcup_{j=1}^{k-1} T^c_{i-1}(\lambda_{j+1}^{i-1}) \right) \cup \left( \bigcup_{j=1}^{k-1} [T^c_{i-1}(\lambda_{j-1}^{i-1}) \setminus G_{i-1}(\lambda_{j-1}^{i-1})] \right)
\]

which implies

\[
t^c_i(\lambda^i) = t^c_{i-1}(\lambda_{0}^{i-1}) + \sum_{j=1}^{k-1} t^c_{i-1}(\lambda_{j+1}^{i-1}) + \sum_{j=1}^{k-1} [t^c_{i-1}(\lambda_{j-1}^{i-1}) - g_{i-1}(\lambda_{j-1}^{i-1})].
\]

We next provide an interpretation of \( G_{i-1}(\lambda_{j-1}^{i-1}) \). Suppose the entry extracted at step \( i \) is \( j(i) \). The fact that \( \alpha \) is in a stack implies that the \((i - 1)\)th step is also a \(-\square\) step and that the extracted entry is \( j(i) + 1 \). For \( \vartheta \in G_{i-1}(\lambda_{j-1}^{i-1}) \), we apply Lemma \( \Box \)and replace the insertion of step \( j(i) + 1 \) and the extraction at step \((i - 1)\) by respective \( \varnothing \)-steps, and thereby obtain the \(*\)-tableaux \( f(\vartheta) \). We then remove the two \( \varnothing \)-steps and obtain the unique \(*\)-tableaux

\( \vartheta' \in T^c_{i-3}(\lambda_{j-1}^{i-3}) \),

where \( \lambda^i \) can be derived from \( \lambda_{j-3}^{i-3} \) by removing a square in the \( j \)th row. We next claim \( \vartheta' \in T^c_{i-3}(\lambda_{j-3}^{i-3}) \setminus G_{i-3}(\lambda_{j-3}^{i-3}) \). Suppose \( \vartheta' \in G_{i-3}(\lambda_{j-3}^{i-3}) \), then \( \vartheta \) contains a stack of length three, implying \( \vartheta \notin G_{i-1}(\lambda_{j-1}^{i-1}) \), which is impossible. Therefore, we have the bijection

\[
\beta: G_{i-1}(\lambda_{j-1}^{i-1}) \longrightarrow T^c_{i-3}(\lambda_{j-3}^{i-3}) \setminus G_{i-3}(\lambda_{j-3}^{i-3}),
\]

from which we conclude

\[
g_{i-1}(\lambda_{j-1}^{i-1}) = t^c_{i-3}(\lambda_{j-3}^{i-3}) - g_{i-3}(\lambda_{j-3}^{i-3}).
\]

Replacing the term \( g_{i}(\lambda_{j-1}^{i}) \) and using the fact that for any shape \( \mu \), \( g_i(\mu) = g_0(\mu) = 0 \) holds, we arrive at

\[
g_{i-1}(\lambda_{j-1}^{i-1}) = \sum_{p=1}^{\lfloor \frac{i-1}{2} \rfloor} (-1)^{p-1} t^c_{i-2p-1}(\lambda_{j-1}^{i-2p-1}).
\]
This allows us to rewrite eq. (2.6) as

\[ t^c_i(\lambda^i) = t^c_{i-1}(\lambda_0^{i-1}) + \sum_{j=1}^{k-1} t^c_{i-1}(\lambda_j^{i-1}) + \sum_{j=1}^{k-1} \sum_{p=0}^{\lfloor (n-i)/2 \rfloor} (-1)^p t_{i-1-2p}^c(\lambda_j^{i-1-2p}) \]

and the proof of the lemma is complete. \( \square \)

Lemma 2 allows us to compute the terms \( t^c_i(\lambda) \) for arbitrary \( i \) and \( \lambda \) recursively via the terms \( t^c_h(\lambda') \), where \( h < i \) and the shapes \( \lambda' \) differ from \( \lambda \) by at most one square.

We next generate a \( \ast \)-tableaux \( \vartheta \in T^c_{n-i}(\lambda^n = \emptyset) \) from right to left. For this purpose we set \( \mu^i = \lambda^{n-i} \) for all \( 0 \leq i \leq n \) and initialize \( \mu^0 = \emptyset \). Suppose we have at step \( i \) the shape \( \mu^i \) and consider the \( T^c_{n-i}(\lambda^{n-i}) \)-paths starting from \( \lambda^0 = \emptyset \) and ending at \( \lambda^{n-i} = \mu^i \).

**Corollary 1.** The transition probabilities

\[ \mathbb{P}(X^{i+1} = \mu^{i+1} \mid X^i = \mu^i) = \begin{cases} \frac{t^c_{n-i-1}(\mu^{i+1})}{\sum_{p=0}^{\lfloor (n-i)/2 \rfloor} (-1)^p t_{n-i-2p-1}^c(\mu^{i+1})} & \mu^i \setminus \mu^{i+1} = +\Box_j, \emptyset \\ \frac{t^{c}_{n-i}(\mu)}{\sum_{p=0}^{\lfloor (n-i)/2 \rfloor} (-1)^p t_{n-i-2p-1}(\mu^{i+1})} & \mu^i \setminus \mu^{i+1} = -\Box_j, \end{cases} \]

where \( 1 \leq j \leq k-1 \), induce a locally uniform Markov-process \( (X^i)_i \) whose sampling paths are shape-sequences \( (\mu^i)_i \).

Let \( \text{Rand}(\mu^i) \) denote the random process of locally uniformly choosing \( X^{i+1} = \mu^{i+1} \) for given \( X^i = \mu^i \) using the transition probabilities given in eq. (2.8). Corollary 1 gives rise to the following algorithm:

The key observation now is that any core-diagram generated via the above Markov process has uniform probability.

**Theorem 1.** Any core-diagram generated via the Markov-process \( (X^i)_i \) (by means of the algorithm \( \text{Rand}(\mu^i) \)) is generated with uniform probability.
Algorithm 1 Core$(n, k)$

1: $m \leftarrow 0$
2: while $m < n$ do
3:   $\mu_{m+1} \leftarrow \text{Rand}(\mu^m)$
4:   if $\mu_{m+1} \setminus \mu^m = +\Box$ then
5:     insert $(m + 1)$ in the new square
6:   else if $\mu_{m+1} \setminus \mu^m = -\Box$ then
7:     let pop be the unique extracted entry of $T^m$ which if RSK-inserted into $T^{m+1}$ recovers $T^m$
8:     create an arc $(pop, m + 1)$
9:     if $(pop, m + 1)$ is stacking with lastpair then
10:        restart the process Core$(n, k)$
11:     else
12:        put $(pop, m + 1)$ in the arc set $A$
13:        lastpair $\leftarrow (pop, m + 1)$
14:   end if
15: end if
16: $m \leftarrow m + 1$
17: end while

Proof. Suppose we are given a sequence of shapes

\[ \mu^i, \mu^{i-1}, \ldots, \mu^0 = \emptyset \]

Let $U_{n-i}(\mu^i)$ denote the subset of $*$-tableaux

\[ \emptyset = \lambda^0, \lambda^1, \ldots, \lambda^{n-i} = \mu^i \]

such that there is no stack in the induced arc set of

\[ (\lambda^0, \ldots, \lambda^{n-i-1}, \lambda^{n-i} = \mu^i, \mu^{i-1}, \ldots, \mu^0 = \emptyset). \]

In particular, $U_n(\emptyset)$ denotes the set of all $*$-tableaux of shape $\emptyset$ having at most $(k - 1)$ rows that generate only core-diagrams. Let $u_n(\emptyset) = |U_n(\emptyset)|$ denote the number of cores of length $n$. By construction, we have

\[ U_{n-i}(\mu^i) \subseteq T^e_{n-i}(\mu^i), \]

\[ u_n(\emptyset) = |U_n(\emptyset)|. \]
We now condition the process \((X^i)_i\), whose transition probabilities are given by eq. (2.8), on generating cores. That is, we consider only those \(*\)-tableaux generated by \((X^i)_i\) that are contained in \(U_n(\emptyset)\). Let this process be denoted by \((Z^i)_i\). We observe

\[
\begin{align*}
(T_{n-i-1}^c(\mu^{i+1}) \setminus G_{n-i-1}(\mu^{i+1})) \cap U_{n-i-1}(\mu^{i+1}) &= U_{n-i-1}(\mu^{i+1}) \\
T_{n-i}^c(\mu^i) \cap U_{n-i}(\mu^i) &= U_{n-i}(\mu^i) \\
T_{n-i-1}^c(\mu^{i+1}) \cap U_{n-i-1}(\mu^{i+1}) &= U_{n-i-1}(\mu^{i+1}).
\end{align*}
\]

Accordingly, using eq. (2.8), we derive for the transition probabilities

\[
\mathbb{P}(Z^{i+1} | Z^i) = \frac{|U_{n-i-1}(\mu^{i+1})|}{|U_{n-i}(\mu^i)|}.
\]

Therefore we arrive at

\[
\mathbb{P}(Z^{i+1}) = \prod_{p=0}^{i} \frac{|U_{n-i+p}(\mu^{i+1-p})|}{|U_{n-i+p}(\mu^{i-p})|} = \frac{|U_{n-i-1}(\mu^{i+1})|}{|U_n(\mu^0 = \emptyset)|} \cdot \frac{|U_{n-i-1}(\mu^{i+1})|}{u_n(\emptyset)}
\]

and in particular

\[
\mathbb{P}(Z^n = \emptyset) = \frac{|U_0(\mu^n = \emptyset)|}{|U_n(\mu^0 = \emptyset)|} = \frac{1}{u_n(\emptyset)},
\]

which implies that the process \((Z^i)_i\) generates cores with uniform probability. \(\Box\)

### 3. Modular diagrams

Any \(\sigma\)-modular diagram can be mapped into a \(\sigma\)-weighted core, i.e. a diagram whose arcs have additional weights \(\geq \sigma\). Suppose we have a \(*\)-tableaux of \(\emptyset\), \(\vartheta\), whose induced diagram is a \(\sigma\)-modular diagram. Repeated application of Lemma \(\Box\) for each respective stack

\[
S = ((p, q), (p + 1, q - 1), \ldots, (p + (s - 1), q - (s - 1)));
\]
allows us to replace any insertion-step $p+1, \ldots, p+(s-1)$ as well as any extraction-step $q-(s-1), \ldots, q-1$ by ∅-steps, respectively. Removing the $2(s-1)$ ∅-steps and assigning the stack-lengths $s$ to the extraction in step $q$, generates a *-tableaux of ∅ with weights, $\theta$ ($\sigma$-weighted *-tableaux).

Using the correspondence between *-tableaux and diagrams, a $\sigma$-weighted core can therefore be represented as a sequence of shapes, $\theta$ in which, preceding each extraction step, we have the additional insertion of exactly $2(s-1)$ ∅-steps, see Fig. 5. Let $W_i^\sigma(\lambda^r)$ denote the set of $\sigma$-weighted *-tableaux. Each such $\theta \in W_i^\sigma(\lambda^r)$ induces a unique *-tableaux, $p(\theta)$, contained in $T_c^r(\lambda^r)$ and we have

$$i = r + \sum_{\ell=1}^{h \leq r/2} 2(s_\ell - 1),$$

where $s_\ell$ is the weight of the $\ell$th extraction in $\theta$. We set $w_i^\sigma(\lambda^r) = |W_i^\sigma(\lambda^r)|$. 

**Figure 5.** (a) a *-tableaux whose induced diagram is a 2-modular diagram. (b) the *-tableaux obtained by repeated application of Lemma 1. The red and blue removed arcs correspond the red and blue ∅-steps in the *-tableaux, respectively. (c) the weighted *-tableaux induced by (b) with weights 2 and 4 assigned to the two extraction steps, respectively, and its induced weighted core.
Lemma 3. We have the recursion formula

\begin{equation}
(3.1) \quad w_i(\lambda^r) = w_{i-1}^\sigma(\lambda_{j-1}^r) + \sum_{j=1}^{k-1} w_{i-1}^\sigma(\lambda_{j+1}^r)
\end{equation}

\begin{equation}
+ \sum_{j=1}^{k-1} \sum_{s=\sigma} \sum_{\ell=1}^{\lfloor \frac{i-1}{s} \rfloor} (-1)^{\ell-1} p(s, \ell, \sigma) w_{i-2s+1}^\sigma(\lambda_{j-1}^r),
\end{equation}

where \( p(a, \ell, \sigma) \) denotes the number of partitions of \( a \) into \( \ell \) blocks, \( \{a_1, a_2, \ldots, a_\ell\} \), such that \( \forall i \leq \ell, a_i \geq \sigma \).

Proof. Any \(*\)-tableaux \( \theta \in W_i^\sigma(\lambda^r) \), where \( i = r + \sum_{\ell=1}^{k} 2(s_{\ell} - 1) \), \( s_{\ell} \) is the weight assigned to the \( \ell \)th extraction step in \( \theta \). We consider the weighted \(*\)-tableaux, \( \theta' \), derived from \( \theta \) by removing the shape in step \( r \). If \( \lambda^r \) is derived from \( \lambda^{r-1} \) by doing nothing, then \( \theta' \in W_{i-1}^\sigma(\lambda_{j-1}^r) \). Similarly, if \( \lambda^r \) is derived from \( \lambda^{r-1} \) by adding a square in the \( j \)th row, we have \( \theta' \in W_{i-1}^\sigma(\lambda_{j+1}^r) \). In case of \( \lambda^r \) being derived from \( \lambda^{r-1} \) via removing a square from the \( j \)th row, we are given an extraction step with associated weight \( s \). Thus,

\( \theta' \in W_{r-1+\sum_{\ell=1}^{k} 2(s_{\ell} - 1)}^\sigma(\lambda_{j-1}^r) = W_{(i-1)-2(s-1)}^\sigma(\lambda_{j-1}^r) \).

\( \theta' \) determines \(*\)-tableaux, \( p(\theta') \in T_{r-1}^c(\lambda_{j-1}^r) \setminus G_{r-1}(\lambda_{j-1}^r) \). Let \( V_{(i-1)-2(s-1)}^\sigma(\lambda_{j-1}^r) \) denote the set of weighted \(*\)-tableaux \( \theta_1 \) such that \( p(\theta_1) \in G_{r-1}(\lambda_{j-1}^r) \). We set \( u_{(i-1)-2(s-1)}^\sigma(\lambda_{j-1}^r) = |V_{(i-1)-2(s-1)}^\sigma(\lambda_{j-1}^r)| \). Note that then \( \theta' \in W_{(i-1)-2(s-1)}(\lambda_{j-1}^r) \setminus V_{(i-1)-2(s-1)}(\lambda_{j-1}^r) \), whence

\begin{equation}
W_i^\sigma(\lambda^r) = W_{i-1}^\sigma(\lambda_{j-1}^r) \cup \left( \bigcup_{j=1}^{k-1} W_{i-1}^\sigma(\lambda_{j+1}^r) \right)
\end{equation}

\begin{equation}
\cup \left( \bigcup_{j=1}^{k-1} \bigcup_{s=\sigma} \left[ W_{(i-1)-2(s-1)}^\sigma(\lambda_{j-1}^r) \setminus V_{(i-1)-2(s-1)}^\sigma(\lambda_{j-1}^r) \right] \right).
\end{equation}
We therefore derive

\[(3.2)\]

\[w_i^\sigma(\lambda^r) = w_i^\sigma(\lambda_0^r) + \sum_{j=1}^{k-1} w_i^\sigma(\lambda_{j+1}^r) + \sum_{j=1}^{k-1} \sum_{s=\sigma}^{i \downarrow} [w_i^\sigma_{2s+1}(\lambda_{j-1}^r) - v_{i-2s+1}^\sigma(\lambda_{j-1}^r)].\]

We proceed by considering a *-tableaux \(\zeta \in V_{(i-1)-2(s-1)}^\sigma(\lambda_{j-1}^r)\). By construction, \((r-1)\) is a \(-\square\)-step. Suppose the induced arc of this extraction is \(\alpha\) and the weight assigned to it is given by \(s'\). Then \(p(\zeta) \in G_{r-1}(\lambda_{j-1}^r)\) and we have the bijection

\[\beta: G_{r-1}(\lambda_{j-1}^r) \longrightarrow T_{r-3}(\lambda_{j-3}^r) \setminus G_{r-3}(\lambda_{j-3}^r),\]

obtained by removing the insertion and extraction step of the extracted square in step \((r-1)\). Taking into the account weights, \(\beta\) gives rise to the bijection

\[\beta': V_{(i-1)-2(s-1)}^\sigma(\lambda_{j-1}^r) \longrightarrow \bigcup_{s' = \sigma}^{i-2+1} [W_{(i-1)-2(s+s'-1)}^\sigma(\lambda_{j-3}^r) \setminus V_{(i-1)-2(s+s'-1)}^\sigma(\lambda_{j-3}^r)],\]

from which we conclude

\[v_{(i-1)-2(s-1)}^\sigma(\lambda_{j-1}^r) = \sum_{s' = \sigma}^{i-2+1} [w_{(i-1)-2(s+s'-1)}^\sigma(\lambda_{j-3}^r) - v_{(i-1)-2(s+s'-1)}^\sigma(\lambda_{j-3}^r)].\]

Using (a)

\[\sum_{s_1 = \sigma}^{i} \cdots \sum_{s_\ell = \sigma}^{i} x_{s_1 + \cdots + s_\ell} = p(s, \ell, \sigma) x_{s}\]

where \(p(s, \ell, \sigma)\) denotes the number of partitions of \(s\) into \(\ell\) blocks of size \(\geq \sigma\), and (b) that for any shape \(\mu\), \(v_1^\sigma(\mu) = v_0^\sigma(\mu) = 0\). We iterate the above formula by
replacing the terms $v^r_i(\lambda^r_{j-})$

\[
\sum_{s=\sigma}^{i+1} (w^r_{i-2s+1}(\lambda^r_{j-}) - v^r_{i-2s+1}(\lambda^r_{j-}))
\]

\[
= \sum_{s=\sigma}^{i+1} w^r_{i-2s+1}(\lambda^r_{j-}) - \sum_{s=\sigma}^{i+1} \sum_{s'=\sigma}^{2i+1} (w^r_{i-2s-2s'+1}(\lambda^r_{j-}) - v^r_{i-2s-2s'+1}(\lambda^r_{j-}))
\]

\[\vdots\]

\[
= \sum_{s_1=\sigma}^{2(s_1+\cdots+s_\ell)\leq i+1} \sum_{s_\ell=\sigma}^{s_\ell} (-1)^\ell w^r_{i-2(s_1+\cdots+s_\ell)+1}(\lambda^r_{-2\ell+1})
\]

\[
= \sum_{s=\sigma}^{i+1} \sum_{\ell=1}^\sigma (-1)^{\ell-1} p(s, \ell, \sigma) w^r_{i-2s+1}(\lambda^r_{j-}),
\]

whence the lemma. \qed

Lemma 3 allows us to compute $w^r_i(\mu)$ for arbitrary $i, \mu$ inductively via the terms $w^r_h(\lambda)$ and $h < i$. We next consider the generation of a $\ast$-tableaux, $\vartheta$, which corresponds to a $\sigma$-modular diagram. For this purpose we shall generate a weighted $\ast$-tableaux $\theta \in W^\sigma_n(\lambda^m = \emptyset)$. Taking the sum over all weights we have $m = n - \sum h 2(s_h - 1)$. We construct $\theta$ inductively from right to left setting $\mu^r = \lambda^{m-r}$. We initialize $\mu^0 = \emptyset$ and assign in case of $\mu^r \setminus \mu^{r+1} = -\emptyset$ a weight to step $r$. Suppose we have arrived at $\mu^r$, with the corresponding set of weights, $S^r$. Considering sequences of weighted $\ast$-tableaux contained in $W^\sigma_{n-r-\sum_{s|\in S^r} 2(s+1)}(\mu^r)$, Lemma 3 implies
Corollary 2. Let
\[ t = n - r - \sum_{s \in S^r} 2(s - 1) \]
\[ z_{\ell-1}^{\sigma}(\mu^r_{j-1}, s) = \sum_{\ell=1}^{s} (-1)^{\ell-1} p(s, \ell, \sigma) w_{\ell-2s+1}^{\sigma}(\mu^r_{j-1}). \]

The transition probabilities
\[ P(X^{r+1} = (\mu^{r+1}, S^{r+1}) | X^r = (\mu^r, S^r)) \]
\[ = \begin{cases} w_{\ell}^{\sigma+1}(\mu^{r+1}) & \mu^r \setminus \mu^{r+1} = +\square_j, S^{r+1} = S^r \\ w_{\ell}^{\sigma}(\mu^r) & \mu^r \setminus \mu^{r+1} = \emptyset, S^{r+1} = S^r \\ z_{\ell-1}^{\sigma}(\mu^{r+1}, s) & \mu^r \setminus \mu^{r+1} = -\square_j, S^{r+1} = S^r \cup \{s\}, \end{cases} \]
for \(1 \leq j \leq k - 1\), generate a locally uniform Markov-process \((X^i)_i\).

Corollary 2 represents an algorithm for constructing \(\sigma\)-modular diagrams. In analogy to the case of core-diagrams, if \(X\) successfully constructs a modular diagram, it generates the latter with uniform probability, see Fig. 2 (left-hand side). Consequently, the process \((X^i)_n\) generates random \(\sigma\)-modular, \(k\)-noncrossing diagram in \(O(n)\) time and space complexity. According to the recursion of Lemma 3 we compute \(w_i^\sigma(\lambda^i)\) for arbitrary \(\lambda^i\) with at most \((k - 1)\) rows and all \(i \leq n\) in \(O(n) \times O(n^{k-1}) = O(n^k)\) time and space complexity.

Theorem 2. Any modular diagram derived via the Markov-process \((X^r)_r\) is generated with uniform probability.

Proof. Suppose we have a sequence of shapes
\[ \mu^r, \mu^{r-1}, \ldots, \mu^0 = \emptyset \]
Algorithm 2 Canonical\((n,k,σ)\)

1: \(m ← 0\)
2: \(\textbf{while } m < n \textbf{ do}\)
3: \((μ^{m+1}, \text{size}) ← \text{RandStep}(μ^m)\)
4: \(\textbf{if } μ^{m+1} \setminus μ^m = +□ \textbf{ then}\)
5:insert \(m + 1\) in the new square
6:assign size to the the new square
7:\(m ← m + \text{size} - 1\)
8: \(\textbf{else if } μ^{m+1} \setminus μ^m = -□ \textbf{ then}\)
9:let \(pop\) be the unique extracted entry of \(T^m\) which if RSK-inserted into \(T^{m+1}\), recovers \(T^m\) and let size be the integer assigned to the extracted square
10:create a stack \(\{(pop, m + \text{size}), \cdots, (pop + \text{size} - 1, m + 1)\}\)
11:\(\textbf{if } (pop, m + \text{size}) \text{ is stacking with lastpair } \textbf{ then}\)
12:restart the process Canonical\((n,k,σ)\)
13: \(\textbf{else}\)
14:put \(\{(pop, m + \text{size}), \cdots, (pop + \text{size} - 1, m + 1)\}\) in the arc set \(A\)
15:lastpair ← \((pop, m + \text{size})\)
16:\(m ← m + \text{size} - 1\)
17: \(\textbf{end if}\)
18: \(\textbf{end if}\)
19:\(m ← m + 1\)
20: \(\textbf{end while}\)

with weights assigned to each \(μ^{i-1} \setminus μ^i = -□_j\)-step and set of weights, \(S^r\). Let
\[
t = n - r - \sum_{s_ℓ ∈ S^r} 2(s_ℓ - 1)
\]
and \(D^r_{m-r}(μ^r)\) be the set of weighted \(*\)-tableaux
\[
λ^0 = ∅, λ^1, \ldots, λ^{m-r} = μ^r
\]
such that
\[
∅ = λ^0, \ldots, λ^{m-r-1}, λ^{m-r} = μ^r, μ^{r-1}, \ldots, μ^0 = ∅
\]
is contained in $W_n^\sigma(\lambda^m = \emptyset)$. Summing over all weights we have $m = n - \sum s_h 2(s_h - 1)$ and by construction, $D_{m-r}^\sigma(\mu^r) \subseteq W_t^\sigma(\mu^r)$. In particular

$$d_m^\sigma(\emptyset) = |D_m^\sigma(\mu^m = \emptyset)|$$

equalsthe number of weighted core of length $m$, i.e. the number of modular diagrams of length $n$. Suppose now we only consider sampling paths of weighed cores generated via $(X^r)_r$ (whose transition probabilities is given by eq. (3.3)) contained in $D_m^\sigma(\emptyset)$. We denote the resulting process by $(Z^r)_r$. In view of

$$(W_{t-1}^\sigma(\mu^{r+1}) \setminus V_{t-1}^\sigma(\mu^{r+1})) \cap D_{m-r-1}^\sigma(\mu^{r+1}) = D_{m-r-1}^\sigma(\mu^{r+1})$$

$$W_t^\sigma(\mu^r) \cap D_m(\mu^r) = D_m(\mu^r)$$

$$W_{t-1}^\sigma(\mu^{r+1}) \cap D_{m-r-1}(\mu^{r+1}) = D_{m-r-1}(\mu^{r+1}).$$

Therefore we have

$$P(Z^{r+1} | Z^r) = \frac{|D_{m-r-1}^\sigma(\mu^{r+1})|}{|D_m^\sigma(\mu^r)|}$$

and consequently

$$P(Z^{r+1}) = \prod_{p=0}^r \frac{|D_{m-r-1+p}^\sigma(\mu^{r+1-p})|}{|D_{m-r+p}^\sigma(\mu^{r-p})|} = \frac{|D_{m-r-1}^\sigma(\mu^{r+1})|}{|D_m(\mu^0 = \emptyset)|}.$$ 

In particular,

$$P(Z^m = \emptyset) = \frac{|D_m^\sigma(\mu^m = \emptyset)|}{|D_m^\sigma(\mu^0 = \emptyset)|} = \frac{1}{|D_m(\mu^0 = \emptyset)|} = \frac{1}{d_m^\sigma(\emptyset)}.$$ 

That is, the process $(Z^r)$ generates modular diagrams uniformly and the theorem follows. 

In Fig. we showcase two paths constructed via the process Canonical$(n, k, \sigma)$, for $n = 8, k = 3$ and $\sigma = 2$. In Fig. we construct the corresponding 2-modular diagram from the red path displayed in Fig. 6.
Figure 6. Building weighted \(\ast\)-tableaux via the transition probabilities given in eq. (3.3). Here, the top path fails to generate a 2-modular diagram while the red path succeeds. According to Theorem 2 each such modular diagram is generated with uniform probability.

(a) \(\emptyset \leftarrow [2/2, 1/2] \leftarrow [1, 1/2] \leftarrow [1] \leftarrow \emptyset\)

(b) \(\emptyset \leftarrow [3/2, 3/2, 1/3, 1/3] \leftarrow [1/3, 1/3] \leftarrow [1/3, 1/3] \leftarrow \emptyset\)

(c) \(\emptyset \leftarrow [3/4, 3/4, 3/3, 3/3] \leftarrow [3/3, 3/3] \leftarrow [3/3, 3/3] \leftarrow \emptyset\)

Figure 7. (a) the red path of Fig. 6. (b) the \(\ast\)-tableaux derived by adding four \(\emptyset\)-steps in (a). (c) adding two pairs of insertion and extraction steps, which produces the 2-modular diagram.

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