Algebraic Systems for DNA Origami Motivated by Jones Monoids

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Overview

1. Introduction
2. Constructing an Origami Monoid
3. Algebraic Structure of Origami Monoid

Monoid Preliminaries

Definition

The free monoid over an alphabet Σ is the set of all finite (possibly empty) strings of symbols from Σ, denoted Σ^*, equipped with string concatenation. The identity element is the empty word, and is written as 1 or ϵ.

Example

For $\Sigma = \{a, b\}$, some elements of Σ^* include 1, a, b, and $aaba$.
$ab \cdot ba = abba$.

Rewriting Preliminaries

Definition

A rewriting system R for alphabet Σ is a subset of $\Sigma^* \times \Sigma^*$, and for $(u, v) \in R$, we write $u \to v$. We may extend these relations by defining $s \underset{R}{\to} t$ if there exist $x, y, u, v \in \Sigma^*$ such that $s = xuy$, $t = xvy$, and $u \to v$.

Example

For $\Sigma = \{a, b\}$ and $R = \{(aa, a), (bb, b), (aba, a), (bab, b)\}$, we have $abab \underset{R}{\to} ab$ since

$\underline{aba}b \underset{R}{\to} \underline{a}b$ and

$a\underline{bab} \underset{R}{\to} a\underline{b}$.

Rewriting Preliminaries

Definition

For Σ with rewriting system R, define a relation $\sim$ on Σ^* by $u \sim v$ if there exist $s_1, s_2, \ldots, s_n \in \Sigma^*$ such that
$u \underset{R}{\rightarrow} s_1 \underset{R}{\rightarrow} \ldots \underset{R}{\rightarrow} s_n \underset{R}{\rightarrow} v$.
We may extend $\sim$ to an equivalence relation $\sim^*$, then $M = \Sigma^*/\sim^*$ is the monoid associated with alphabet Σ and rewriting system R.

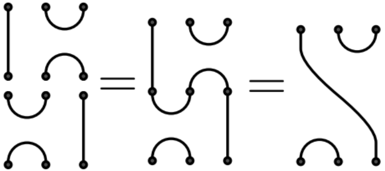
Example

For $\Sigma = \{a, b\}$ and $R = \{(aa, a), (bb, b), (aba, a), (bab, b)\}$,
$M = \Sigma/\sim^* = \{[1], [a], [b], [ab], [ba]\}$.
$[a] = [aa] = [aaa] = [aba] = [aababa]$.
$[a] \cdot [ab] = [aab] = [ab]$.

Jones Monoids

- $\mathcal{J}_n$ has generators $h_1, \ldots, h_{n-1}$

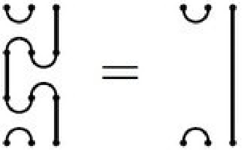
- Define multiplication by vertical concatenation



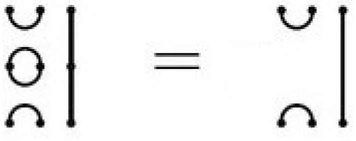
Abramsky, S., Temperley-Lieb algebra: from knot theory to logic and computation via quantum mechanics. arXiv:0910.2737 (2009)

Jones Monoids

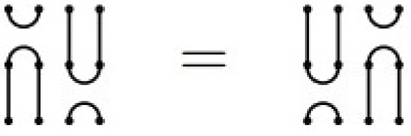
- 3 types of rewriting rules:
  - $h_i h_j h_i \rightarrow h_i$, $|i-j| = 1$
  - $h_i h_i \rightarrow h_i$
  - $h_i h_j \rightarrow h_j h_i$, $|i-j| \geq 2$



$h_1 h_2 h_1 = h_1$



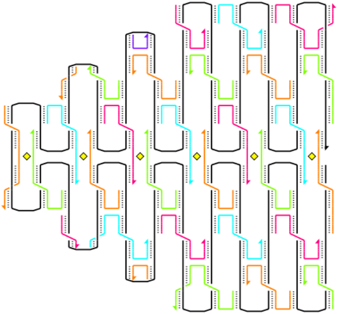
$h_1^2 = h_1$

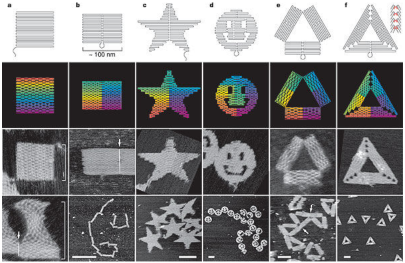


$h_1 h_3 = h_3 h_1$

DNA Origami

- Create complex structures at a nano-level
- Long, folded single-stranded DNA scaffold strand (black)
- Many short connecting staple strands (color)

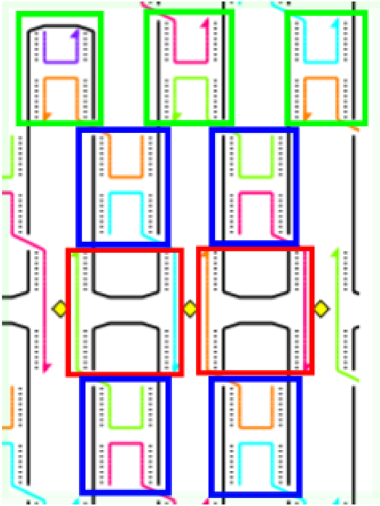




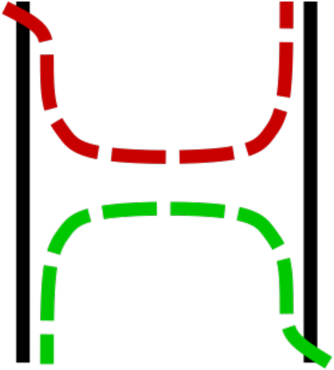
Rothemund, P. W. *Folding DNA to Create Nanoscale Shapes and Patterns*. Nature, 440. 297-302 (2006).

Building Blocks of DNA Origami

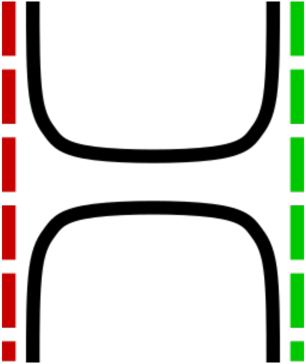
- Common patterns in DNA origami



Identified Building Blocks



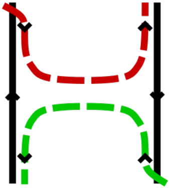
α



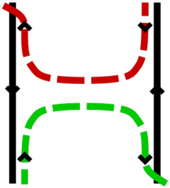
β

Generators for an Origami Monoid

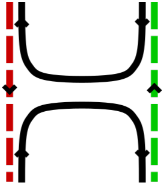
- n — number of vertical scaffold strands
- Index $i = 1, \ldots, n-1$ indicating location of α or β
- Direction varies with parity of i



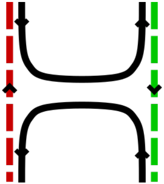
α_i, i odd



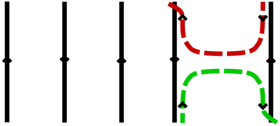
α_i, i even



β_i, i odd



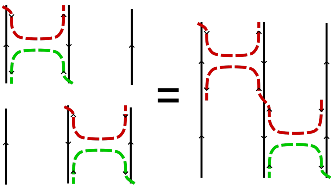
β_i, i even



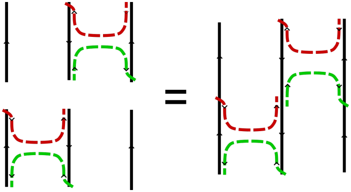
Ex: α_4, $n = 6$

Concatenation of Origami Generators

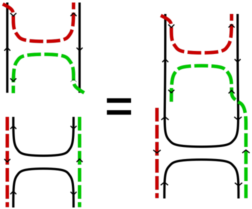
- Line up and connect scaffold
- Connect staples following original diagram



$\alpha_i \alpha_{i+1}$



$\alpha_i \alpha_{i-1}$

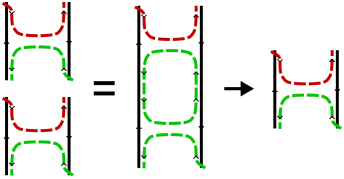


$\alpha_i \beta_i$

Rewriting Rules for DNA Origami

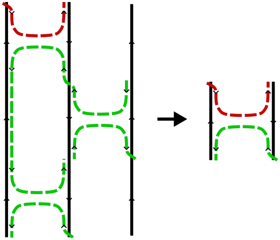
For $\gamma \in \{\alpha, \beta\}$:

(1) $\gamma_i\gamma_i \to \gamma_i$



Ex: $\alpha_i\alpha_i \to \alpha_i$

(2) $\gamma_i\gamma_j\gamma_i \to \gamma_i$, $|i-j| = 1$

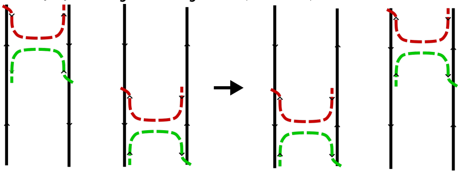


Ex: $\alpha_i\alpha_{i+1}\alpha_i \to \alpha_i$

Rewriting Rules for DNA Origami

For $\gamma \in \{\alpha, \beta\}$ and $\overline{\alpha} = \beta$, $\overline{\beta} = \alpha$:

(3) $\gamma_i \gamma_j \to \gamma_j \gamma_i$, $|i - j| \geq 2$



Ex: $\alpha_i \alpha_{i+2} \to \alpha_{i+2} \alpha$

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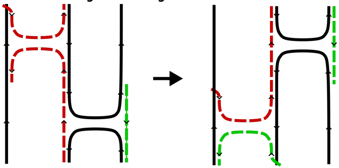
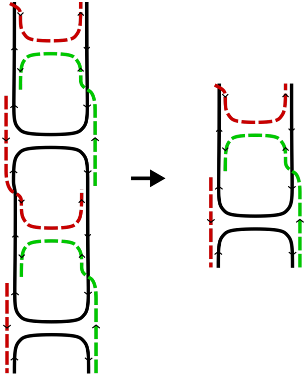
(4) $\gamma_i \overline{\gamma}_j \to \overline{\gamma}_j \gamma_i$, $|i - j| \geq 1$



Ex: $\alpha_i \beta_{i+1} \to \beta_{i+1} \alpha_i$

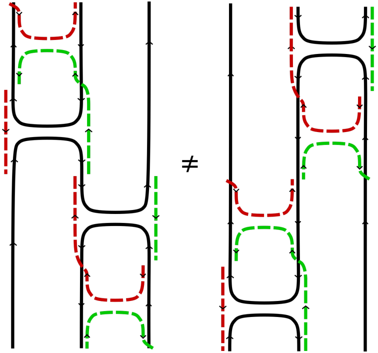
Substitution Rewriting Rules

In addition, we consider $\gamma \in \{\alpha\beta, \beta\alpha, \alpha\beta\alpha, \beta\alpha\beta\}$



$\gamma = \alpha\beta$ in (1)

$\alpha_i\beta_i\alpha_i\beta_i \to \alpha_i\beta_i$



$\gamma = \alpha\beta$ in (4)

$\alpha_i\beta_i\beta_{i+1}\alpha_{i+1} \not\to \beta_{i+1}\alpha_{i+1}\alpha_i\beta_i$

Definition of Origami Monoid $\mathcal{O}_n$

Definition

For $n \in \mathbb{N}$, define $\mathcal{O}_n$ to be the monoid generated by $\alpha_1, \ldots, \alpha_{n-1}, \beta_1, \ldots, \beta_{n-1}$ with relations generated by rewriting rules of $\gamma \in \{\alpha, \beta\}$ for (1) – (4) and $\gamma \in \{\alpha\beta, \beta\alpha, \alpha\beta\alpha, \beta\alpha\beta\}$ for (1) – (2).

(1) $\gamma_i\gamma_i \to \gamma_i$

(2) $\gamma_i\gamma_j\gamma_i \to \gamma_i$, $|i-j| = 1$

(3) $\gamma_i\gamma_j \to \gamma_j\gamma_i$, $|i-j| \geq 2$

(4) $\gamma_i\overline{\gamma}_j \to \overline{\gamma}_j\gamma_i$, $|i-j| \geq 1$

Connections to Jones Monoid

Definition

Define $\mathcal{O}_n^{\alpha}$ to be the submonoid of $\mathcal{O}_n$ generated by αs, and similarly for $\mathcal{O}_n^{\beta}$. Define $\mathcal{O}_n^{\alpha\beta} = [\mathcal{O}_n \backslash (\mathcal{O}_n^{\alpha} \cup \mathcal{O}_n^{\beta})] \cup \{1\}$.

Lemma

$\mathcal{J}_n \cong \mathcal{O}_n^{\alpha} \cong \mathcal{O}_n^{\beta}$.

Proof.

If $h_1, \ldots h_{n-1}$ are the generators of $\mathcal{J}_n$, define a map $p_{\alpha} : \mathcal{O}_n \to \mathcal{J}_n$ by $p_{\alpha}(\alpha_i) = h_i$ and $p_{\alpha}(\beta_i) = 1$. Define p_{β} similarly by $p_{\beta}(\alpha_i) = 1$ and $p_{\beta}(\beta_i) = h_i$. Observe that p_{α} and p_{β} are monoid morphisms, and that $p_{\alpha}|_{\mathcal{O}_n^{\alpha}}$ and $p_{\beta}|_{\mathcal{O}_n^{\beta}}$ are bijections. □

Connections to Jones Monoid

Definition

Define $p : \mathcal{O}_n \to \mathcal{J}_n \times \mathcal{J}_n$ by $p(u) = (p_\alpha(u), p_\beta(u))$.

Lemma

p is an onto monoid morphism.

Structure $\mathcal{O}_n$ for $n \leq 6$

We use computer program GAP to study $\mathcal{O}_n$ for small n

n	$\lvert\mathcal{J}_n\rvert$	$\lvert\mathcal{J}_n\rvert^2$	$\lvert\mathcal{O}_n\rvert$
2	2	4	7
3	5	25	45
4	14	196	294
5	42	1764	2180
6	132	17424	19087

The GAP Group, *GAP – Groups, Algorithms, and Programming, Version 4.9.3*; 2018, (www.gap-system.org).

Elements of $\mathcal{O}_3$

$1, \alpha_1, \alpha_2, \beta_1, \beta_2, \alpha_1\alpha_2, \alpha_1\beta_1, \alpha_1\beta_2, \alpha_2\alpha_1, \alpha_2\beta_1, \alpha_2\beta_2, \beta_1\alpha_1,$
$\beta_1\beta_2, \beta_2\alpha_2, \beta_2\beta_1, \alpha_1\alpha_2\beta_1, \alpha_1\alpha_2\beta_2, \alpha_1\beta_1\alpha_1, \alpha_1\beta_1\beta_2, \alpha_1\beta_2\alpha_2,$
$\alpha_1\beta_2\beta_1, \alpha_2\alpha_1\beta_1, \alpha_2\alpha_1\beta_2, \alpha_2\beta_1\alpha_1, \alpha_2\beta_1\beta_2, \alpha_2\beta_2\alpha_2, \alpha_2\beta_2\beta_1,$
$\beta_1\alpha_1\alpha_2, \beta_1\alpha_1\beta_1, \beta_1\alpha_1\beta_2, \beta_1\beta_2\alpha_2, \beta_2\alpha_2\alpha_1, \beta_2\alpha_2\beta_1, \beta_2\alpha_2\beta_2,$
$\beta_2\beta_1\alpha_1, \alpha_1\alpha_2\beta_1\beta_2, \alpha_1\alpha_2\beta_2\beta_1, \alpha_1\beta_1\beta_2\alpha_2, \alpha_2\alpha_1\beta_1\beta_2, \alpha_2\alpha_1\beta_2\beta_1,$
$\alpha_2\beta_2\beta_1\alpha_1, \beta_1\alpha_1\alpha_2\beta_2, \beta_1\alpha_1\beta_2\alpha_2, \beta_2\alpha_2\alpha_1\beta_1, \beta_2\alpha_2\beta_1\alpha_1$

Green's Classes

Definition

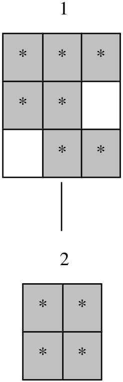
For monoid M, define equivalence relations $\mathscr{L}$, $\mathscr{R}$, $\mathscr{D}$, $\mathscr{H}$ on M by
$a \mathscr{L} b$ if there exist $x, y \in M$ such that $xa = b$ and $yb = a$,
$a \mathscr{R} b$ if there exist $x, y \in M$ such that $ax = b$ and $by = a$,
$a \mathscr{D} b$ if there exists $c \in M$ such that $a \mathscr{L} c$ and $c \mathscr{R} b$, and
$a \mathscr{H} b$ if $a \mathscr{L} b$ and $a \mathscr{R} b$.

The equivalence classes of these relations are Green's $\mathscr{L}$, $\mathscr{R}$, $\mathscr{D}$, and $\mathscr{H}$ classes, respectively.

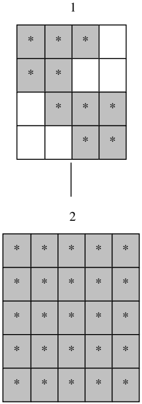
- $\mathscr{L}$ and $\mathscr{R}$ can also be described by principal ideals.
- In a finite monoid, $\mathscr{D}$-classes correspond to two-sided principal ideals.

Green's Classes for Jones Monoid

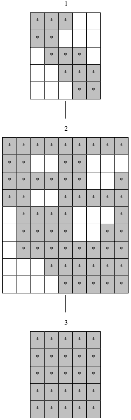
- $\mathscr{L}$ – *classes*: columns
- $\mathscr{R}$ – *classes*: rows
- $\mathscr{D}$ – *classes*: big boxes
- $\mathscr{H}$ – *classes*: small boxes



$\mathcal{J}_4$



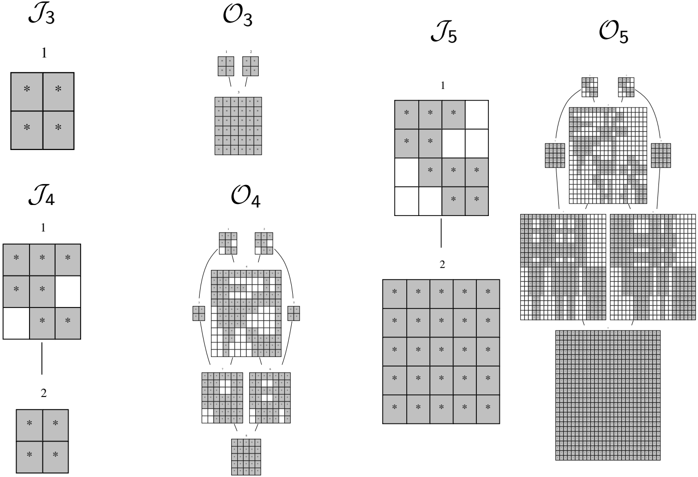
$\mathcal{J}_5$



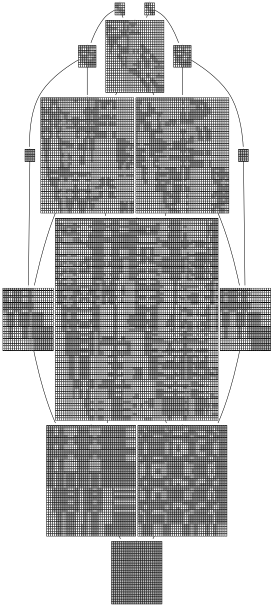
$\mathcal{J}_6$

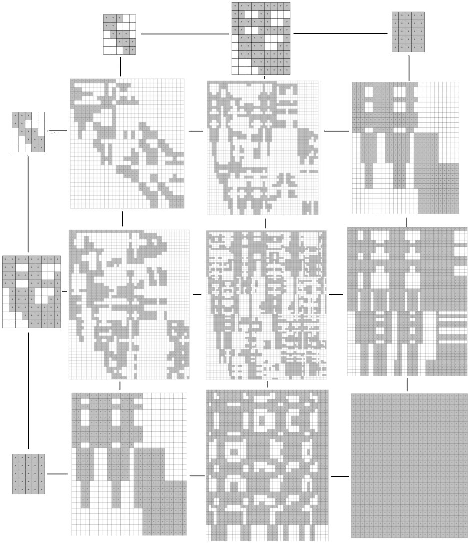
Relation Between Green's Classes of $\mathcal{O}_n$

- 2 copies of $\mathscr{D}$-classes of $\mathcal{J}_n$ in $\mathcal{O}_n$
- Other $\mathscr{D}$-classes of $\mathcal{O}_n$ correspond to $\mathscr{D}$-classes of $\mathcal{J}_n \times \mathcal{J}_n$



Relation Between Green's Classes of $\mathcal{O}_n$, $n = 6$





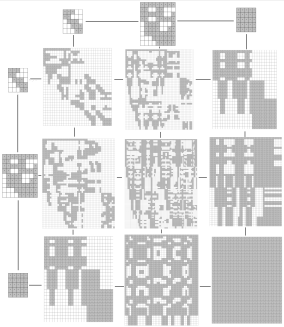
Conjectures for General $\mathcal{O}_n$

Conjecture

$\mathcal{O}_n$ is finite for all n.

Conjecture

For every $\mathscr{D}$-class D of $\mathcal{J}_n \times \mathcal{J}_n$, there exists a unique $\mathscr{D}$-class D' of $\mathcal{O}_n$ such that $p(D') = D$.



Acknowledgements

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