On the power of oritatami cotranscriptional folding with unary bead sequence*

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Abstract. We investigate simple oritatami systems in an attempt to establish lower bounds on the size and complexity of computationally universal systems. In particular, we look at oritatami systems, where the folding sequence consists of a number of beads of the same type and show that under reasonable assumptions, these systems are not universal.

1 Introduction

Transcription is the first essential step of gene expression, in which a DNA template sequence is copied into a complementary single stranded RNA sequence by a 'copy machine' called RNA polymerase. The RNA strand is synthesized letter by letter according to the complimentarity relation $\mathtt{A} \to \mathtt{U}$, $\mathtt{G} \to \mathtt{C}$, $\mathtt{C} \to \mathtt{G}$, and $\mathtt{T} \to \mathtt{A}$ and folds up during a process called co-transcriptional folding.

In a recent breakthrough in molecular engineering by Geary, Rothemund and Andersen [5] the co-transcriptional folding of RNA is controlled by careful design of the DNA template. As demonstrated in laboratory, this method, called RNA Origami, makes it possible to build rectangles out of RNA strands. Geary et al. [3] proposed a mathematical model for this process, called oritatami system. It has been just shown in [4] that the model is efficiently Turing universal by simulating cyclic tag systems introduced by Cook [1]. The simulation involves a very large and complex oritatami system. One future direction of research is to find smaller universal oritatami system.

Closely related is the question of where not to look for universal systems, i.e., what are the limitations of simple oritatami system. In search for simple oritatami systems, there are a number of restrictions one can pose on them:

- bounds on the delay, the number of bead types or the arity;
- bounds on the size of the primary structure or of the attraction rule set;

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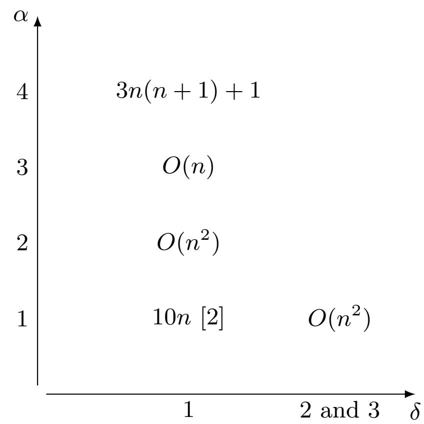


Fig. 1. Summary of the results.

– structural conditions on the primary structure or the attraction rule set.

In this paper we start a new line of study which concerns the alphabet size for the primary structure, i.e., the number of bead types.

2 Preliminaries

Let Σ be a set of types of abstract molecules, or *beads*. A bead of type $a \in \Sigma$ is called an a-bead. By Σ^* and Σ^ω, we denote the set of finite sequences of beads and that of one-way infinite sequences of beads, respectively. The empty sequence is denoted by λ. Let $w = b_1 b_2 \cdots b_n \in \Sigma^*$ be a sequence of length n for some integer n and bead types $b_1, \dots, b_n \in \Sigma$. The *length* of w is denoted by $|w|$, that is, $|w| = n$. For two indices i, j with $1 \leq i \leq j \leq n$, we let $w[i..j]$ refer to the subsequence $b_i b_{i+1} \cdots b_{j-1} b_j$; if $i = j$, then $w[i..i]$ is simplified as $w[i]$. For $k \geq 1$, $w[1..k]$ is called a *prefix* of w.

Oritatami systems fold their transcript, which is a sequence of beads, over the triangular grid graph $\mathbb{T} = (V, E)$ cotranscriptionally. We designate one point in V as the origin O of $\mathbb{T}$. For a point $p \in V$, let $\varhexagon_p^d$ denote the set of points which lie in the regular hexagon of radius d centered at the point p. Note that $\varhexagon_p^d$ consists of $3d(d+1)+1$ points. A directed path $P = p_1 p_2 \cdots p_n$ in $\mathbb{T}$ is a sequence of *pairwise-distinct* points $p_1, p_2, \dots, p_n \in V$ such that $\{p_i, p_{i+1}\} \in E$ for all $1 \leq i < n$. Its i-th point is referred to as $P[i]$. Now we are ready to abstract RNA single-stranded structures in the name of conformation. A *conformation* C (over Σ) is a triple (P, w, H) of a directed path P in $\mathbb{T}$, $w \in \Sigma^*$ of the same length as P, and a set of h-interactions $H \subseteq \big\{\{i, j\} \bigm| 1 \leq i, i+2 \leq j, \{P[i], P[j]\} \in E\big\}$. This is to be interpreted as the sequence w being folded along the path P in such a manner that its i-th bead $w[i]$ is placed at the i-th point $P[i]$ and the i-th and j-th beads are bound (by a hydrogen-bond-based interaction) if and only if $\{i, j\} \in H$. The condition $i+2 \leq j$ represents the topological restriction that two consecutive beads along the path cannot be bound. The *length* of C is defined to be the length of its transcript w (that is, equal to the length of the path P). A *rule set* $R \subseteq \Sigma \times \Sigma$ is a symmetric relation over Σ, that is, for all bead types $a, b \in \Sigma$, $(a, b) \in R$ implies $(b, a) \in R$. A bond $\{i, j\} \in H$ is *valid with respect to* R, or simply R-valid, if $(w[i], w[j]) \in R$. This conformation C is *R-valid* if all of its bonds are R-valid. For an integer $\alpha \geq 1$, C is *of arity* α if it contains a bead that forms α bonds but none of its bead forms more. By $\mathcal{C}_{\leq\alpha}(\Sigma)$, we denote the set of all conformations over Σ whose arity is at most α; its argument Σ is omitted whenever Σ is clear from the context.

The oritatami system grows conformations by an operation called elongation. Given a rule set R and an R-valid conformation $C_1 = (P, w, H)$, we say that another conformation C_2 is an elongation of C_1 by a bead $b \in \Sigma$, written as $C_1 \xrightarrow{R}_b C_2$, if $C_2 = (Pp, wb, H \cup H')$ for some point $p \in V$ not along the path P and set $H' \subseteq \big\{\{i, |w|+1\} \bigm| 1 \leq i < |w|, \{P[i], p\} \in E, (w[i], b) \in R\big\}$ of bonds formed by the b-bead; this set H' can be empty. Note that C_2 is also R-valid. This operation is recursively extended to the elongation by a finite sequence of beads as: for any conformation C, $C \xrightarrow{R}{}^{*}_{\lambda} C$; and for a finite sequence of beads $w \in \Sigma^*$ and a bead $b \in \Sigma$, a conformation C_1 is elongated to a conformation C_2 by wb, written as $C_1 \xrightarrow{R}{}^{*}_{wb} C_2$, if there is a conformation C' that satisfies $C_1 \xrightarrow{R}{}^{*}_{w} C'$ and $C' \xrightarrow{R}_b C_2$.

An *oritatami system* (OS) $\Xi = (\Sigma, R, \delta, \alpha, \sigma, w)$ is composed of

- a set Σ of bead types,
- a rule set $R \subseteq \Sigma \times \Sigma$,
- a positive integer δ called the *delay*,
- a positive integer α called the *arity*,
- an initial R-valid conformation $\sigma \in C_{\leq\alpha}(\Sigma)$ called the *seed*, upon which
- its (possibly infinite) *transcript* $w \in \Sigma^* \cup \Sigma^\omega$ is to be folded by stabilizing beads of w one at a time so as to minimize energy collaboratively with the succeeding $\delta-1$ nascent beads.

The energy of a conformation $C = (P, w, H)$, denoted by $\Delta G(C)$, is defined to be $-|H|$; the more bonds a conformation has, the more stable it gets. The set $\mathcal{F}(\Xi)$ of conformations *foldable* by the system Ξ is recursively defined as: the seed σ is in $\mathcal{F}(\Xi)$; and provided that an elongation C_i of σ by the prefix $w[1..i]$ be foldable (i.e., $C_0 = \sigma$), its further elongation C_{i+1} by the next bead $w[i+1]$ is foldable if

$$C_{i+1} \in \mathop{\arg\min}_{\substack{C \in \mathcal{C}_{\leq\alpha} s.t. \\ C_i \xrightarrow{R}_{w[i+1]} C}} \min\Big\{\Delta G(C') \Bigm| C \xrightarrow{R}{}^{*}_{w[i+2 \ldots i+k]} C', k \leq \delta, C' \in \mathcal{C}_{\leq\alpha}\Big\}. \quad (1)$$

Then we say that the bead $w[i+1]$ and the bonds it forms are *stabilized* according to C_{i+1}. Note that an arity-α oritatami system cannot fold any conformation of arity larger than α. A conformation foldable by Ξ is *terminal* if none of its elongations is foldable by Ξ. The oritatami system Ξ is *deterministic* if for all $i \geq 0$, there exists at most one C_{i+1} that satisfies (1). A deterministic oritatami system folds into a unique terminal conformation. An oritatami system with the empty rule set just folds into an arbitrary elongation of its seed nondeterministically. Thus, the rule set is always assumed to be non-empty.

In this paper, we considerably focus on the unary oritatami system. An oritatami system is *unary* if its bead type set Σ is of size 1. Its sole bead type is denoted by a, that is, $\Sigma = \{a\}$. Its only possible rule is (a, a) so that the non-empty rule set assumption implies that its rule set is $R = \{(a, a)\}$. Its transcript is a sequence of a-beads. That is to say, the behavior of a unary oritatami system is fully determined by the delay, arity, and seed.

Proposition 1. *For any rule set R, arity α and conformation $C = (P, w, H)$ it is possible to check whether C is R-valid and whether $C \in \mathcal{C}_{\leq\alpha}$ in time $\mathcal{O}(|H| \cdot |w| \cdot |R|)$.*

Proof. To check whether C is R-valid:

1. FOR each $(i, j) \in H$:
2. IF $(w[i], w[j]) \notin R$ THEN answer NO and HALT
3. answer YES and HALT

Checking the condition in 2. can be done in $\mathcal{O}(|w| \cdot |R|)$ time for any reasonable representation of w and R, hence the whole process takes $\mathcal{O}(|H| \cdot |w| \cdot |R|)$ time. To check the arity constraint $C \in \mathcal{C}_{\leq\alpha}$:

1. FOR each $i \in \{1, \ldots, |w|\}$:
2. IF degree$(i) = |\{j | (i, j) \in H\}| > \alpha$ THEN answer NO and HALT
3. answer YES and HALT

Checking the condition in 2. can be done in $\mathcal{O}(|H|)$ time for any reasonable representation of H, hence the whole process takes $\mathcal{O}(|w| \cdot |H|)$ time.

Theorem 1. *There is an algorithm that simulates any oritatami system $\Xi = (\Sigma, R, \delta, \alpha, \sigma, w)$ in time $2^{\mathcal{O}(\delta)} \cdot |R| \cdot |w|$.*

Proof. Take any step in the computation, up to which some $i \geq 0$ first beads of w have been stabilized, with the last bead at a point p. The number of all possible elongations of the current conformation by the next δ-beads is $(6 \times 5^{\delta-1}) \times ((2^4)^{\delta-1} \times 2^5) \in 2^{O(\delta)}$. By Proposition 1, we can check for each of these elongations whether its arity is at most α or not and whether it is R-valid or not in time $\mathcal{O}((2^4)^{\delta-1} \cdot 2^5 \cdot \delta \cdot |R|) = 2^{\mathcal{O}(\delta)} \cdot |R|$. Therefore, the total running time is $2^{\mathcal{O}(\delta)} \cdot |R| \cdot |w|$.

Corollary 1. *For fixed δ and α, the class of problems solvable by oritatami systems $(\Sigma, R, \delta, \alpha, \sigma, w)$ is included in* DTIME(n^3).

Proof. The claim follows from Theorem 1 and the fact that $|R|$ is implicitly bounded by $|w|^2$.

Because of the time hierarchy theorems, we know that P $\subsetneq$ EXP, so we can conclude that OS which cannot deterministically fold transcripts of length exponential in the length of the seed are not computationally universal.

3 Problem description

In [2], Demaine et al. proved that at delay 1 and arity 1, upon the seed of length n, a deterministic oritatami system cannot fold into any conformation strictly longer than $10n$. We consider this finiteness problem for unary oritatami systems under various settings of the values of delay and arity, which is formalized as follows.

Problem 1. Give an upper bound on the length of a transcript of a delay-δ, arity-α deterministic unary oritatami system whose seed is of length n by a function in δ, α, and n.

Results on this problem are summarized in Fig. 1.

4 Case of arity 1

4.1 $\alpha = 1$, arbitrary alphabets

First we present a lower bound construction for arity $\alpha = 1$ systems. At $\alpha = 1$, allowing delay $\delta = 2$ increases the power of OS compared with $\delta = 1$, if at least four bead types are allowed. We demonstrate this with an infinite family of OS, which fold deterministically a transcript of length $\frac{(n-1)^2}{4}$ starting from a given seed of length n.

Consider the following $\delta = 2$, $\alpha = 1$ system with bead types $\{0, 1, 2, 3, 4\}$ and attraction rules $\{(1,1), (2,2), (3,3), (4,4)\}$. Let the seed σ be a conformation of a $4k+1$ long bead sequence of the form $(1020)^k 0$, such that bead $\sigma[i]$ of the seed is stabilized at point $(i, 0)$, for all $1 \le i \le 4k-1$. Bead $4k$ is at $(4k-1, -1)$ and bead $4k+1$ is at $(4k, 0)$.
The transcript is

$$
w = \begin{array}{ll}
k \text{ odd} & k \text{ even} \\
(2413)^{k-1}241 & (2413)^{k-1}241 \\
(4231)^{k-1}4 & (4231)^{k-1}4 \\
(1324)^{k-2}132 & (1324)^{k-2}132 \\
(3142)^{k-2}3 & (3142)^{k-2}3 \\
(2413)^{k-3}241 & (2413)^{k-3}241 \\
(4231)^{k-3}4 & (4231)^{k-3}4 \\
(1324)^{k-4}132 & (1324)^{k-4}132 \\
(3142)^{k-4}3 & (3142)^{k-4}3 \\
\vdots & \vdots \\
(2413)^{2}241 & (2413)^{1}241 \\
(4231)^{2}4 & (4231)^{1}4 \\
(1324)^{1}132 & (1324)^{0}132 \\
(3142)^{1}3 & (3142)^{0}3 \\
(2413)^{0}241 & \\
(4231)^{0}4 &
\end{array}
$$

The transcript above is written in rows which correspond to beads in the conformation stabilized along the same row on the grid. To simplify the argument we will use *row* both for the transcript above and for the conformation it stabilizes in. In line with this, row $\ell \in \{1, \dots, 2k\}$ is as follows:

row ℓ	$\ell \mod 4$
$(2413)^{k-\lfloor(\ell+1)/2\rfloor}241$	$\ell \equiv 1 \mod 4$
$(4231)^{k-\lfloor(\ell+1)/2\rfloor}4$	$\ell \equiv 2 \mod 4$
$(1324)^{k-\lfloor(\ell+1)/2\rfloor}132$	$\ell \equiv 3 \mod 4$
$(3142)^{k-\lfloor(\ell+1)/2\rfloor}3$	$\ell \equiv 4 \mod 4$

so $w = \mathrm{row}_1 \cdots \mathrm{row}_{2k}$. Row 1 is of length $4k-1$ and row $\ell+1$ is two beads shorter than row ℓ, so the length of the whole transcript is $|w| = 4k^2 = \frac{(4k+1-1)^2}{4} = \frac{(|\sigma|-1)^2}{4}$. As an example, see Fig. 2, where $k = 5$, so the length of the seed is $4k+1 = 21$ and the transcript is $4k^2 = 100$ beads long.

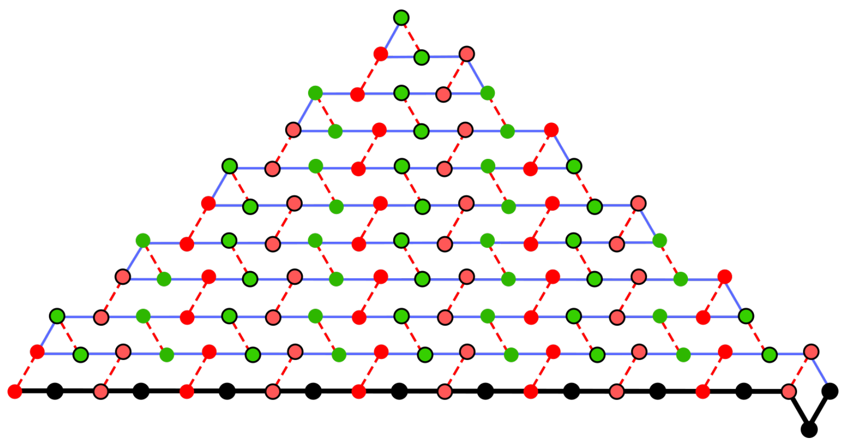
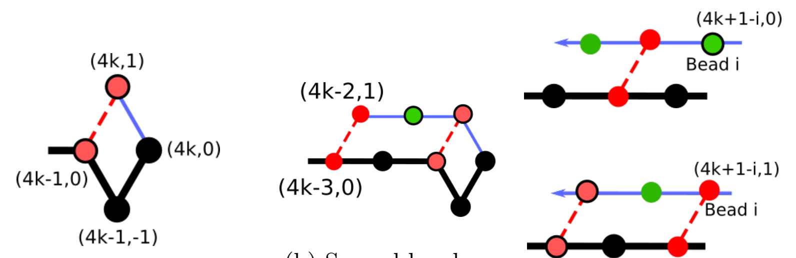


Fig. 2. Quadratic length transcript folding deterministically into pyramid shape. Seed: thick black path. Transcript: thin blue path. Bonds: dashed red lines. Beads: '0' black, '1' red, '2' red with black contour, '3' green, '4' green with black contour.

Stabilizing the first bead of row j goes as follows (see Fig. 4):

$j \mod 4$	first bead	predecessor at	first bead binds to	first stabilizes at
$\equiv 1$	2	$(4k - \frac{j-1}{2}, j-1)$	$(4k - \frac{j+1}{2}, j-1)$	$(4k - \frac{j+1}{2}, j)$
$\equiv 2$	4	$(\frac{3j}{2} - 1, j-1)$	$(\frac{3j}{2}, j-1)$	$(\frac{3j}{2}, j)$
$\equiv 3$	1	$(4k - \frac{j-1}{2}, j-1)$	$(4k - \frac{j+1}{2}, j-1)$	$(4k - \frac{j+1}{2}, j)$
$\equiv 4$	3	$(\frac{3j}{2} - 1, j-1)$	$(\frac{3j}{2}, j-1)$	$(\frac{3j}{2}, j)$



(a) First transcript bead

(b) Second bead

(c) Bead $i+1$, when bead i is $B_{3,4}$ and $B_{1,2}$, respectively

Fig. 3. Fixing transcript beads in odd rows

As for the other beads, in rows $j \equiv 1,3 \mod 4$, beads of type 1 and 3 bind to a bead in row $j-1$. In rows $j \equiv 2,4 \mod 4$ beads of type 2 and 4 can bind to a bead in row $j-1$. This is true for row 1, because beads of type 1 and 3 from row 1 can only bind to every second bead of the seed, whereas beads of type 2 and 4 from row 1 cannot bind to anything (Fig. 3, (c)). Once this dynamic holds for a row, it holds inductively for the next, as a bead that binds to another loses its only free hand at arity 1.

Within one row of the transcript, no bead can bind to a preceding bead, because if there is a previous bead of the same type in that row, it is stabilized at a distance of four and the system has delay 2.

By the arguments above, the beads in row i of the transcript are stabilized along row i on the grid, forming the pyramid-like conformation from Fig. 2.

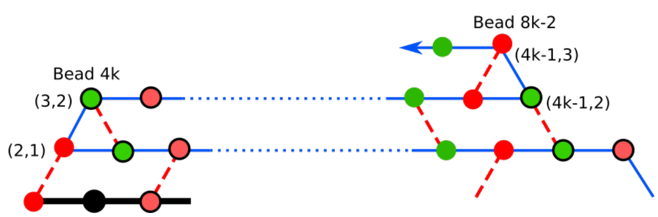


Fig. 4. Beads $4k, 8k-2, \ldots$ stabilize at turning points because the bead two positions before is the same type and has a free hand.

4.2 $\alpha = 1$, unary

Let the point where the first transcript bead was fixed be p and let $n = |\text{seed}|+1$. We will argue about the situation when the first bead is stabilized outside $\hexagon_p^n$ (a hexagon of radius n). Let this be the ith bead of the transcript. Without loss of generality, we can translate the origin $(0,0)$ to the coordinates of bead $i-1$

(which is still in $\hexagon_p^n$), and we can assume that the bead outside the hexagon is fixed at $(1,1)$ (see Fig. 5).

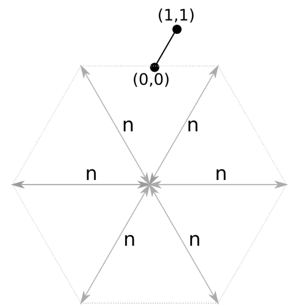
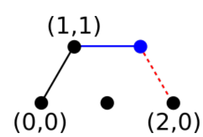


Fig. 5. $\hexagon_p^n$ and the position $(1,1)$ of the first bead fixed outside of it.

In the elongation that places bead i at $(1,1)$ there are two possibilities:

- i forms a bond with a bead at $(1,0)$.
- i does not bond to anything and $i+1$ is at $(2,1)$ bonding with a bead at $(2,0)$. If there is no bead at $(1,0)$, then placing i at $(1,0)$ instead of $(1,1)$ results in the same number of bonds, leading to nondeterminism. Therefore, there has to be a bead at $(1,0)$ and it is inactive, otherwise it would bond to i. This is analogous to case 1. below.



The next bead, $i+1$, can be fixed at $(2,1)$ or at $(0,1)$ as all other possibilities result in nondeterministic behavior immediately, so we have two cases.

1. bead $i+1$ is fixed at $(2,1)$ and can bond with a bead at $(2,0)$. Now consider bead $i+2$. For $i+1$ to be fixed at $(2,1)$, $i+2$ needs to form a bond somewhere, otherwise $i+2$ could go to $(2,1)$ forming the bond with the bead at $(2,0)$ and there would be two conformations with the maximal 1 bond. The only possibility is that there is a bead at $(3,0)$ and $i+2$ can bond with it when placed at $(3,1)$. We can apply the same argument inductively: there is some $m \geq 0$ such that grid points $(\ell,0)$ are occupied by active beads, for all $\ell \in \{2,\ldots,2+m\}$, and there is no bead at $(3+m,0)$. Such an m exists, and it is not greater than n. Then, bead $i+\ell$ is fixed at $(\ell+1,1)$ and bonds with $(\ell+1,0)$. However, bead $i+2+m$ cannot be fixed anywhere, because

$i+2+m$ and $i+3+m$ can only add one bond to the conformation, and that is possible either with $i+2+m \to (2+m,1)$, $i+3+m \to (3+m,1)$ or with $i+2+m \to (2+m,2)$, $i+3+m \to (2+m,1)$.

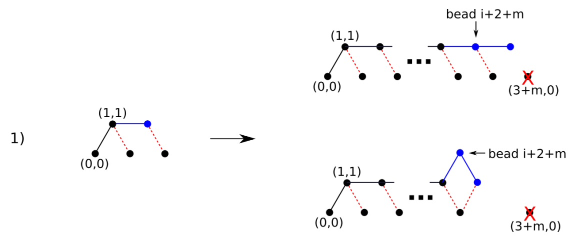


Fig. 6.

2. bead $i+1$ is fixed at $(0,1)$. This is only possible if
   (a) there is an inactive bead at $(-1,0)$ and an active one at $(-2,0)$. This case is symmetrical to (1).
   (b) there is no bead at $(-1,0)$, bead $i+1$ can bond with bead $i-1$ at $(0,0)$ and the bead $i+2$ can be placed at $(-1,0)$ where it can bond with $(-2,0)$, $(-2,-1)$ or $(-1,-1)$. This leads to nondeterminism, because bead i at $(-1,0)$ and bead $i+1$ at $(0,1)$ has two bonds, just as the original conformation.
   (c) there is a bead at $(-1,0)$ and bead $i+1$ can bond with that or with bead $i-1$ at $(0,0)$. However, this means that placing bead i at $(0,1)$ at bead $i+1$ at $(1,1)$ creates the same number of hydrogen bonds, thus resulting in bead i not being placed deterministically.

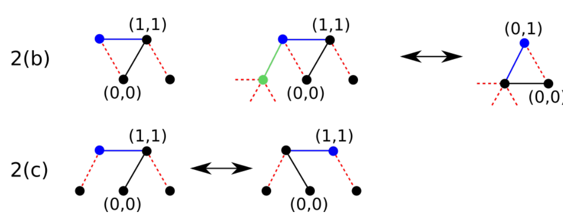


Fig. 7.

4.3 In the case of $\delta = 3$

As before, the length of seed is n and the seed will be inside $\hexagon_p^n$, the equilateral hexagon with a radius of n and center p, the point where the first bead of the seed is fixed. We will begin our discussion by considering the moment when the first bead is fixed outside $\hexagon_p^n$. Let this bead be the ith one.

A. First, let us assume that a fixed bead on a side of $\hexagon_p^n$ has a free hand, and bead i binds to it. If the most stable conformation formed by beads $i, i+1, i+2$ has only two hydrogen bonds, it will be nondeterministic because there are at least two possibilities, see Fig. 8. Therefore, it needs to make three hydrogen bonds to deterministically stabilize i.

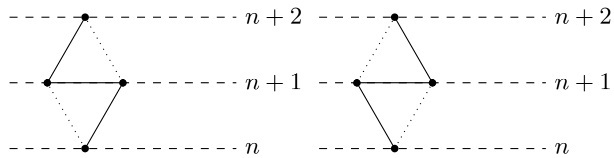


Fig. 8.

There are the two cases in which beads $i, i+1, i+2$ can have three bonds, see Fig. 9. However, if it makes three bonds once, such as in Fig. 9, it will need to make three bonds forever to be deterministic. Similarly to case 1. in the previous section, this becomes nondeterministic finally, as in Fig. 10, when it reaches a corner of $\hexagon_p^n$. Thus, the fixed bead on the side of an equilateral hexagon with a radius of n has to make a hydrogen bond with a bead in an equilateral hexagon.

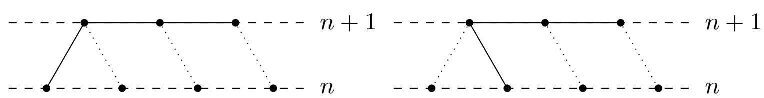


Fig. 9.

B. Next, assume that bead i could not bind to anything and let us discuss the moment after bead i is fixed outside $\hexagon_p^n$. Now bead i has a free hand. If beads $i+1, i+2, i+3$ can form only two bonds, it will be nondeterministic because there are at least two possible such structures, as in Fig. 11. Hence, they need to form three bonds to deterministically stabilize, such as in the right or left side of Fig. 12.

If they form three bonds once, such as Fig. 12, the system would need three bonds forever to be deterministic. This becomes nondeterministic finally, such as in Fig. 10, when it reaches a corner of $\hexagon_p^n$.

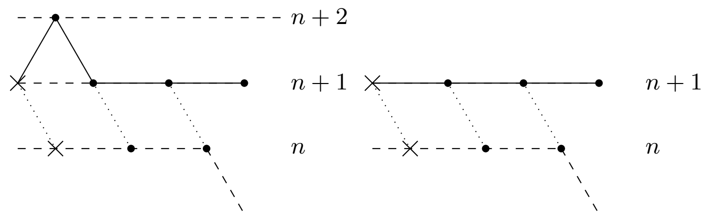


Fig. 10.

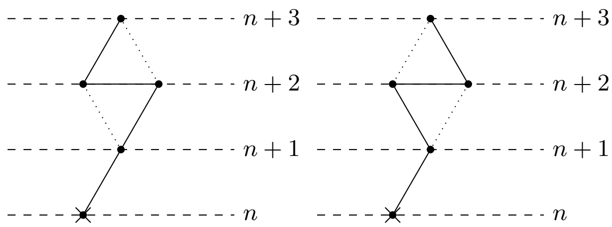


Fig. 11.

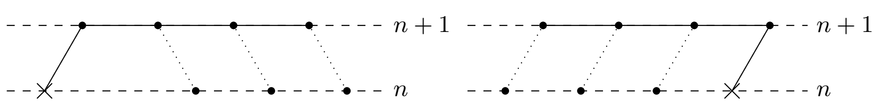


Fig. 12.

Accordingly, it is Fig. 13 when a first bead is fixed on a side of an equilateral hexagon with a radius of $n + 1$.

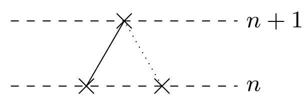


Fig. 13.

5 Case of delay 1

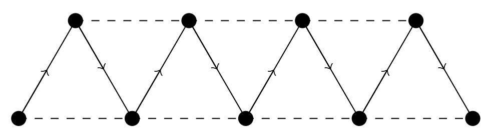


Fig. 14. zig-zag conformation

In this section, we consider Problem 1 at delay 1. Our result, cases of arity 1 and 3 can only yield finite structures of size $O(n)$, and cases of arity 4 and more can only yield finite structures which is size of $O(n^2)$, and a case of arity 2 can yield infinite structures but they are only the zig-zag conformation shown in Fig. 14.

Let $\Xi = (\Sigma, R, \delta, \alpha, \sigma, w)$ be a deterministic oritatami system of delay 1. For $i \geq 0$ let C_i be the unique elongation of σ by $w[1..i]$, that is, foldable by Ξ. Hence $C_0 = \sigma$.

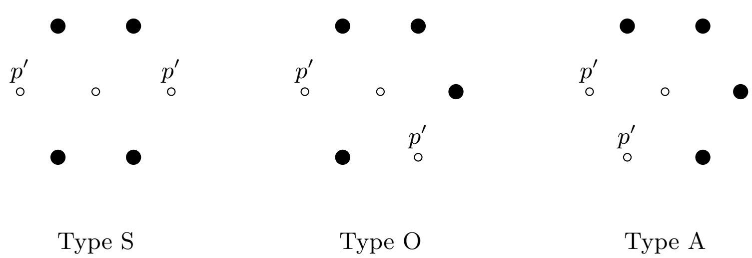


Fig. 15. Tunnel sections of all possible three types: straight (Type S), obtuse turn (Type O), and acute turn (Type A).

At delay 1, a bead cannot collaborate with its successors in order to stabilize itself. In fact, there are just two ways for a bead to get stabilized at delay 1 (or the bead has no place to be stabilized around so that the system halts), as observed in [2]. One is to be bound and the other is through a 1-in-1-out structure called the tunnel section. See Fig. 15. A *tunnel section* consists of four beads that occupy four neighbors of one free point. In order for an oritatam system to stabilize the bead $w[i]$ at the central point p of a tunnel section, its predecessor $w[i-1]$ must be put at one of the two free neighbors of p. Thus, at the stabilization of $w[i]$, only one neighbor of p is left free so that the successor $w[i+1]$ is to be stabilized there, even without being bound. In this case, the point where $w[i-1]$ is stabilized is considered to be an *entrance of the tunnel* and the point where $w[i+1]$ is stabilized is considered as an *exit of the tunnel*.

The behavior of an oritatami system at delay 1 can be described by a sequence of S of b (bound), t_s (straight tunnel section), t_o (obtuse-turn tunnel section), and t_a (acute-turn tunnel section); priority is given to tunnel, that is, $S[i]$ is t_s (resp. t_o, t_a) if the i-th bead of the system is stabilized not only by being bonded but also through a straight (resp. obtuse-turn, acute-turn) tunnel section. We let S take the value $\blacksquare$ for halt (due to the lack of free neighbors).

We say that a neighbor of a point p is reachable from a conformation C if there exists an elongation of C in which a bead occupies the neighbor and it binds with a bead at p. Taking this reachability into account, we define the *binding capability* of a conformation as the number of free bonds of its beads available geometrically for elongations of C. It is defined formally as follows:

Definition 1 (Binding Capability). *Let α be an arity and $C = (P, w, H)$ be a conformation of arity at most α. Let $H_k = H \cap \{(i,j) \mid i = k \text{ or } j = k\}$. Moreover, let R_k be a set of neighbors of the point $P[k]$ that are free and reachable from C. The binding capability of C at arity α, denoted by $\#bc_\alpha(C)$, is defined by $\sum_{k=1}^{|w|} \min\{\alpha - |H_k|, |R_k|\}$. Whenever the arity is clear from context, we omit the subscript α.*

Theorem 2 (Tunnel Troll Theorem). *Let Ξ be a deterministic unary oritatami system of delay $\delta = 1$. At arity $\alpha \geq 3$, if $S[k] = t$ and $S[k+1] \neq \blacksquare$, then $\#bc(C_{k-1}) > \#bc(C_k)$. On the other hand, at arity $\alpha = 2$, if there are indices i, j such that $S[i..j+1]$ is either $bbt^{(j-i-1)}b$ or $bt^\ell bt^{j-i-1-\ell}b$ for some ℓ, then $\#bc(C_{i-1}) > \#bc(C_j)$.*

Lemma 1. *Let Ξ be a deterministic unary oritatami system at delay $\delta = 1$, arity $\alpha = 2$. Assume Ξ stabilizes the transcript until $w[i-1]$. If $S[i+1] = b$ and $S[i+2] \in \{t_s, t_o\}$, then $\#bc(C_{i-1}) > \#bc(C_i)$.*

Proof. See Fig.16. $S[i+2] \in \{t_s, t_o\}$ means that $w[i+2]$ is stabilized by a tunnel section of type S or O. Thus, its predecessor $w[i+1]$ must be inside the tunnel section, that is, n_1 and n_2 must be occupied. Free bonds of $w[i]$, if any, cannot be used in future by another bead $w[j]$ because otherwise the part of transcript $w[i..j]$ and the bond between $w[i]$ and $w[j]$ would form a closed curve and the curve would cross the path of C_{i-1} between n_1 and n_2, contradiction. Therefore, if $w[i]$ forms a bond at its stabilization $\#bc(C_{i-1}) > \#bc(C_i)$ holds. We now prove that $w[i]$ must form a bond.

Suppose $w[i]$ ware stabilized without any bond, that is, by a tunnel. For that the two points that are a neighbor of both $w[i-1]$ and $w[i]$ must be occupied already. In addition, at least one of the neighbors of $w[i]$ must be free because $S[i+1] = b$. Thus, only the case to be considered is Fig. 16 (middle) with n_5 being occupied (that is, n_4 is free). In this case, before $w[i]$ is stabilized, at lest three neighbors of n_2 ware free and hence, a bead at n_2 was provided with one free bond and could form a bond with $w[i]$. □

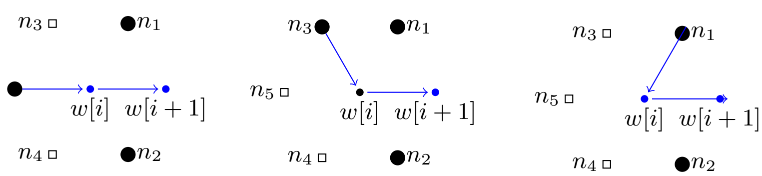


Fig. 16. Direction into a entrance

Lemma 2. *Let Ξ be a deterministic unary oritatami system of delay $\delta = 1$ and arity $\alpha = 2$. If $S[h..i+1] = bt^{(i-h)}b$ for some $h < i-1$, then $\#bc(C_{i-2}) \geq \#bc(C_i)$, and hence, $\#bc(C_{h-1}) \geq \#bc(C_i)$. If $h < i-1$, then the second inequality is strengthened as $\#bc(C_{h-1}) > \#bc(C_i)$.*

Proof. Since the binding capability never increases inside a tunnel, we just need to consider the exit of a tunnel. See Fig.17. At least one of points n_1 or n_2 must be free because otherwise $w[i]$ would be inside of a tunnel, that is, $S[i+1]$ would not be b.

Let a be the number of bonds $w[i-1]$ forms, that is, $\#bc(C_{i-2}) - \#bc(C_{i-1}) = a$. Then, $\#bc(C_i) - \#bc(C_{i-1}) \leq a$ as follows.

- Case of both n_1 and n_2 being free
  This case can be regarded the same as entrance. See Fig.17 (Left). Predecessor n_5 has to be bound to n_4 and n_5 because both of n_3 and n_4 have binding capabilities. Hence, $a \geq 2$. This time, $\alpha = 2$, that is, this case $\#bc(C_i) - \#bc(C_{i-1}) \leq a$.
- Case of n_1 is occupied
  See Fig.17 (Right). If n_1 is occupied, then n_2 is free so that n_5 has to be bound n_4. Hence, $a \geq 1$. This case can supply two binding capabilities but p' can bind to only one of n_0 or n_2 because n_0 or n_2 will be occupied by the successor of p'. Therefore, this case $\#bc(C_i) - \#bc(C_{i-1}) \leq a$.

Thus,$\#bc(C_{i-2}) \geq \#bc(C_i)$, and hence, $\#bc(C_{h-1}) \geq \#bc(C_i)$. If $h < i-1$, then the second inequality is strengthened as $\#bc(C_{h-1}) > \#bc(C_i)$ because $S[h] = b$, that is, $\#bc(C_{h-1}) > \#bc(C_h)$ and $\#bc(C_h) \geq \#bc(C_i)$. □

Point n_1 and n_2 are free

Point n_1 is occupied

Fig. 17. Exit of Tunnel

Lemma 3. *Let Ξ be a deterministic unary oritatami system of delay $\delta = 1$, arity $\alpha = 2$. If there are indices i, j such that $S[i..j+1]$ is either $bbt^{(j-i-1)}b$ and $S[i+2] = t_a$ or $bt^{\ell}bt^{j-i-1-\ell}b$ for some ℓ and $S[i+l+2] = t_a$, then $\#bc(C_{i-1}) > \#bc(C_j)$.*

Proof (Lemma 3). Let Ξ be a unary oritatami system at $\delta = 1, \alpha = 2$. Assume $S[h..i+1] = bt^{i-h}b(h < i)$. If at least one of $w[h+1..i]$ are stabilized by tunnel C, then only $w[h+1]$ can use tunnel C because if $w[g]$ which is one of $w[h+2..i]$, with $h+2 \leq g \leq i$ is stabilized by tunnel C, C_g is a terminal.

Let us consider stabilization $S[h-1..h+1] = tbt$ or $S[h-1..h+1] = bbt$ as follows. In result, $\#bc(C_{h-3}) > \#bc(C_{h+1})$. In addition according to Lemma 2 $\#bc(C_{h+1}) \geq \#bc(C_i)$. Thus, $\#bc(C_{h-3}) > \#bc(C_{h+1})$ and $\#bc(C_{h-3}) > \#bc(C_i)$.

Case of $S[h-1..h+1] = bbt$ See Fig. 18. If $w[h-1]$ forms one bond, then it leaves one free bond, but it is consumed by $w[h+1]$. In addition, $w[h]$ has to bound. Thus, in this cases, binding capability decreases by 1. If $w[h-1]$ forms two bonds, then it does not leave any bond. In addition, $w[h]$ has to be bound. Thus, in this case, even if $w[h+1]$ supplies two free bonds, binding capability decreases by 1.

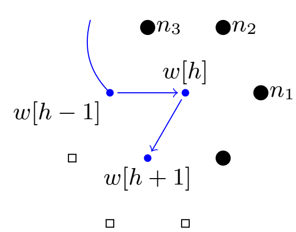
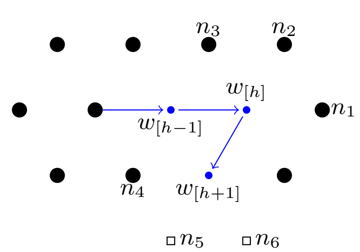


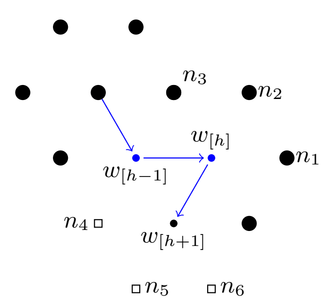
Fig. 18. Case of $S[h-1..h+1] = bbt$

Case of $S[h-1..h+1] = tbt$ Fig.19 exhibits all the two kinds of stabilization depending on structures of tunnel C.

- Left of Fig.19
  In this figure, Bead n_4 has at least one binding so that $w[h-1]$ has to bound n_4. Moreover, $w[h]$ has to bind to one of n_1, n_2, n_3 in order to stabilize deterministically. On the other hand, $w[h+1]$ can supply two bindings but has only two free neighbors. One of them is occupied by a successor. Therefore $w[h+1]$ can only bind one of n_5, n_6, that is, $w[h+1]$ supplies at most one binding. Thus, this case $\#bc(C_{h-1}) > \#bc(C_{h+1})$.
- Right of Fig.19
  These cases are divided on number of capabilities that $w[h-1]$ consumes.
  - $w[h-1]$ does not consume any bindings
    According to Lemma 2, $\#bc(C_{h-3}) \geq \#bc(C_{h-1})$ because of $S[h-1] = t$. $w[h]$ has to bound one of n_1, n_2, n_3 in order to stabilize deterministically so that $\#bc(C_{h-1}) > \#bc(C_h)$. $w[h+1]$ has to be bound to $w[h-1]$ because $w[h-1]$ has bindings, that is, $w[h+1]$ consumes at least one hand and supplies at most one hand so that $\#bc(C_h) \geq \#bc(C_{h+1})$. Thus, in this cases $\#bc(C_{h-3}) > \#bc(C_{h+1})$.
  - $w[h-1]$ consumes one binding
    In this case, w_h has to be bound one of n_1, n_2, n_3. In addition, $w[h-1]$ and $w[h+1]$ are not supply any bindings. Thus, in this cases consume some binding capabilities.
  - $w[h-1]$ consumes two bindings
    In this case, $w[h-1]$ already consumes two binding. $w[h]$ has to be bound. $w[h+1]$ supplies two bindings. Thus, in this cases $\#bc(C_{h-1}) >$ $\#bc(C_{h+1})$.



Pattern 1



Pattern 2

Fig. 19. Case of $S[h-1..h+1] = tbt$

Proof. Each bead in the transcript is bound either inside a tunnel or outside. If a bead is stabilized inside a tunnel, then it has at most one free neighbor, and hence its successor it to be stabilized there. Moreover, if a bead is stabilized outside a tunnel, then its position is either an entrance of a tunnel or not.

Tunnel sections have three possible shapes up to symmetry : straight(S), obtuse(O) and acute(A) turn (Fig. **??**), and we will consider each of those.

Let us first consider cases of $\delta \geq 3, \alpha = 1$. See Fig. 17. Consider the stabilization of $w[i]$. This bead $w[i]$, once stabilized, shares two neighbors with its predecessor $w[i-1]$, which are denoted by n_3, n_4. Both of them have been already occupied because $S[i] = t$.

Since $S[i+1] \neq \blacksquare$, at least one of the other three neighbors, denoted by n_0, n_1, n_2, must be free. Assume that in the neighborhood of $w[i]$, there are two beads with one free neighbor even after $w[i]$ is stabilized. Before the stabilization of $w[i]$, such a bead had two free neighbors, and hence, is provided with at least one free bond. Thus, $w[i]$ is to be bonded to these two beads, and it decreases the binding capability by at least 1. It now suffices to check that this assumption holds no matter how n_0, n_1, n_2 are occupied as long as at least one of them is left free.

Next, we consider the case of $\delta = 2, \alpha = 1$. We assume there is an index h such that $S[h-1..h+1] = bbt$ or $S[h-1..h+1] = tbt$. According to Lemma 1, if $w[h+1]$ is stabilized by tunnel A or B, then $\#bc(C_{h-1}) > \#bc(C_h)$. Also, According to Lemma 3, if $w[h+1]$ is stabilized by tunnel C, then $\#bc(C_{h-3}) > \#bc(C_{h+1})$. On the other hand, if $S[k..l] = bt^{l-k}b$, then $\#bc(C_{k-1}) \geq \#bc(C_l)$ because of Lemma 2. Therefore, if there are indices i and j such that $S[i..j+1] = bbt^{(j-i-1)}b$ or $S[i..j+1] = bt^m bt^n b \quad (m+n = j-i-1)$, then $\#bc(C_{i-1}) > \#bc(C_j)$.

□

5.1 On structures provided by a unary and $\delta = 1$ oritatami system

Theorem 3 **($\delta = 1, \alpha = 2$).** *Let Ξ be a unary oritatami system of $\delta = 1, \alpha = 2$. It can yield infinite structures but they are only zig-zag conformation.*

Proof. By Tunnel Troll Theorem, any tunnel sections which represented in bbt^+ or bt^+bt^+ consume binding capabilities. If the sequence S is free from any subsequence of the form bt^+bt^+, then it can factorize as $S = u_1u_2u_3\cdots$ for some $u_1, u_2, u_3, \cdots \in \{b\} \cup bbt^+$. Assume the length of σ is n, seed supplies at most $2n$ binding capabilities. Therefore formula 2 hold.

$$\exists i \in \mathbb{N} \quad s.t. \quad u_{i-1}, u_i, u_{i+1}, u_{i+2}, \cdots \in \{b\} \tag{2}$$

Let us represent S as $S[i.i+1...] = v_i v_{i+1} v_{i+2} \cdots$ for some $v_i, v_{i+1}, v_{i+2}, \cdots \in \{a, o\}$ where if v_k is a, then v_{k+1} is bound to v_{k-1}, if v_k is o, then v_{k+1} is NOT bound to v_{k-1}.

Let us consider the case of v_k is o. See Fig.20. $w[i-1]$ consumes some binding capabilities because v_{i-1} is b. If the number of $w[i-1]$'s bindings is one binding, then $w[i+1]$ has to be bound except n_1 or n_2 so that $w[i+1]$ must consumes two bindings except the case of n_1 and n_2 are occupied and $w[i]$ consumes at least one binding. If n_1 and n_2 are occupied, then $w[i-1]$'s bindings are inactive, that is, $w[i-1]$ consumes two binding capabilities. Therefore, this case consumes binding capabilities. If $w[i-1]$ dose Not have any bindings, then $w[i-1]$ already consumes two bindings. In addition, $w[i]$ and $w[i+1]$ consume at least one binding. Therefore this case consumes binding capabilities. Thus, the formula 3 hold and according to the formula 2 and the formula 3, the formula 4 is hold. Thus, in this case, oritatami system can yield infinite structures but they are only zig-zag conformation.

$$\exists j \in \mathbb{N} \quad s.t. \quad u_j, u_{j+1}, u_{j+2}, \cdots \in \{a\} \tag{3}$$

$$|S| > \forall m \in \mathbb{N} \quad \rightarrow \quad \exists n \in \mathbb{N} \quad s.t. \quad S[n], S[n+1], \cdots \in \{a\} \tag{4}$$

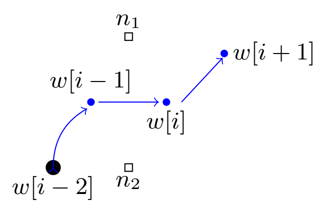


Fig. 20. Case of $S[i]$

Theorem 4 **($\delta = 1, \alpha = 3$).** *Let Ξ be a unary oritatami system of $\delta = 1, \alpha = 3$. It can yield only finite structures whose size is $O(n)$.*

Lemma 4. *Let p be a point whose neighbors is occupied at least two point. If $w[i]$ is not stabilized and $w[i-1]$ includes neighbors of p, then $w[i]$ is stabilized at p with at least one bond, $w[i]$ is stabilized at another point of p otherwise with at least two bond except any neighbors of p is occupied.*

Proof (proof of lemma). Assume the transcript is stabilized until $w[i-1]$. One of neighbors of p is not $w[i-1]$ where this bead regards n_1. If $w[i-1]$ include neighbors of p and $w[i]$ is stabilized at another point of p with one bond. Then, any neighbors do not have bond without $w[i-1]$. Neighbors of n_1 have to be occupied at least five according to lemma **??** and two of them include neighbors of p where each of them regards n_2, n_3. In the same way, five neighbors of n_2 and n_3 are occupied and each of one of them includes neighbors of p where they regard n_4, n_5. one of n_5's neighbors includes neighbors of p where it regards n_6. Then, any neighbors of p are occupied. That is, if some neighbors of p are free, then there exists a bead which has bonds in neighbors.

Proof. Let us show that $\#bc(C_{i-1}) > \#bc(C_i)$, that is, when $w[i]$ is stabilized, $w[i]$ uses at least two hands. Let us assume $w[i]$ is able to be stabilized with using one hand. Fig.21 exhibits all the three kinds of possibility of stabilized $w[i]$. Then, $w[i]$ can be also stabilized at n_3.

Case of straight

- Case of n_3 is free
  According to assumption, $w[i]$ uses only one hand. Therefore, any neighbors of n_3 are occupied according to the lemma4. n_3 and the point which is stabilized $w[i]$ are free so that n_1 has some bond by lemma**??**. Accordingly, this situation is non-deterministic. Thus, n_3 and n_4 have to be occupied because of symmetry.
- Otherwise
  Because of $S[i] = b$, at least one of n_1 and n_2 have to be free. Let us regard that n_1 is free. Neighbors of n_1 have to be occupied and at least two neighbors of n_{-1} have to be free for n_1 and $w[i]$. According to lemma**??**, n_{-1} have some hand. Therefore $w[i]$ can be also stabilized n_1, that is, this situation is non-deterministic. Thus, one of n_3 and n_4 has to be free.

Therefore, this case is false.

Case of obtuse

- Case of n_3 is free
  Any neighbors of n_3 have to be occupied but the point which is stabilized $w[i]$ is free. Thus n_3 has to be occupied.
- Case of n_4 is free
  According to lemma4, n_2 has to be occupied because n_4 is free. Also n_0 has to be occupied from lemma**??**. Thus, only one of n_0, n_3 leave some hands or both of them do not leave any hands because $w[i]$ use only one bond.
  If n_0 has some hands, then n_3 does not have any hands so that n_{-3} is occupied. Also n_{-3} must not have any hands so that n_{-2} is occupied and also n_{-1} is occupied. Therefore any neighbors of $w[i]$ are occupied so that $w[i+1]$ cannot provide.
  If n_3 has some hands, then n_0 does not have any hands so that n_{-1} is occupied. In the same previous way, any n_{-2}, n_{-3} are occupied. Therefore any neighbors of $w[i]$ are occupied.
  If both of n_0, n_3 do not have any hands, then both of n_{-1}, n_{-3} are occupied. If one of n_{-1}, n_{-3} has some hands, the other does not have any hands so that n_{-2} is occupied. If both of n_{-1}, n_{-3} do not have any hands, n_{-2} has to be occupied and n_{-2} has some hands.Therefore any neighbors of $w[i]$ are occupied so that $w[i+1]$ cannot provide.
  Thus n_3 has to be occupied in order to yield infinite structures.
- Case of n_2 is free
  Any neighbors of n_2 have to be occupied so that n_0 is occupied. Any neighbors of n_0 except n_2 have to be also occupied but the point which is stabilized $w[i]$ is free. Thus n_2 has to be occupied.

- Case of n_0 is free
  Any neighbors of n_0 have to be occupied so that n_{-1} is occupied. Any neighbors of n_{-1} except n_0 have to be also occupied but the point which is stabilized $w[i]$ is free. Thus n_0 has to be occupied.

Therefore, any situations contradict $S[i] = b$.

Case of acute

- Case of n_4 is free
  n_4 and a point which is stabilized $w[i]$ are free so that $w[i-2]$ has some hands according to lemma**??**. However, $w[i]$ can be also stabilized n_4 in this case. Thus, n_4 has to be occupied.
- Case of n_2 is free
  According to lemma4, n_0 has to be occupied. n_1 has to be also occupied because of lemma**??**. We consider this case just like case of obtuse and that n_4 is free. Then if $w[i-2]$ binds $w[i]$, any n_{-1}, n_{-2}, n_{-3} are occupied. If n_1 binds $w[i]$, this case is same. Also if n_1 and $w[i-2]$ do not have any hand, any n_{-1}, n_{-2}, n_{-3} are occupied. Therefore, $w[i+1]$ cannot be provided.
- Case of n_0 is free
  Any neighbors of n_0 have to be occupied so that n_1 is occupied. Any neighbors of n_1 except n_0 have to be also occupied but the point which is stabilized $w[i]$ is free. Thus n_0 has to be occupied.
- Case of n_1 is free
  Any neighbors of n_1 have to be occupied so that n_{-1} is occupied. Any neighbors of n_{-1} except n_1 have to be also occupied but the point which is stabilized $w[i]$ is free. Thus n_1 has to be occupied.

Therefore, any situations contradict $S[i] = b$.

Hence, assumption that w[i] is able to be stabilized with using one hand is false. Therefore, when w[i] is stabilized, w[i] uses at least two hands.

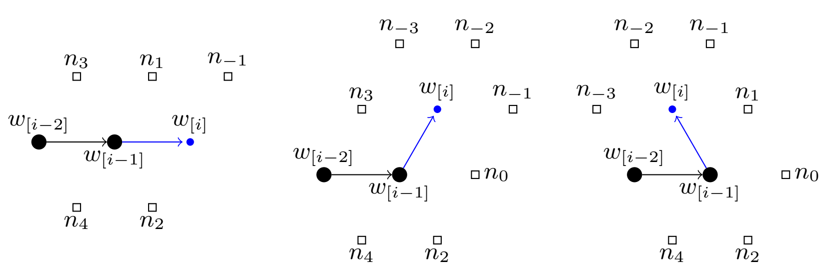


Fig. 21. All possible directions of $w[i]$: straight, obtuse, acute.

Theorem 5 **($\delta = 1, \alpha = 4$).** *Let Ξ be a unary oritatami system of $\delta = 1, \alpha = 4$. It can yield only finite structures whose size is $O(n^2)$.*

Lemma 5. *Any beads which are already stabilized by some bonds use at least two bonds.*

Proof (proof of lemma). Let us consider when $w[i]$ is stabilized by only one bond. See Fig.22. According to lemma**??**, if n_3 is free, $w[i-2]$ has some hands. Thus, n_4 has to be occupied in order to stabilize deterministically. Moreover, also n_2 has to be occupied for deterministic and also n_0, n_1. n_1 has some hands because n_3 is free. Therefore, $w[i]$ is stabilized at n_3 and it has to use at least two hands. It contradict assumption.

Proof. According to lemma5, when $w[i]$ is stabilized, it has to use at least two bonds. Let us consider when a bead $w[i]$ which is the first bead out of $\hexagon^{n}_{w[-n+1]}$ is stabilized. See Fig.23. any n_0, n_1, n_3, n_5 is free because if some of them is occupied, $w[i]$ is not the first bead out of $\hexagon^{n}_{w[-n+1]}$. At least two neighbors of $w[i]$ except predecessor have to be occupied in order to bind. In this case, a point which is able to put a bead is only n_2. Therefore, any transcript cannot be stabilized in out of $\hexagon^{n}_{w[-n+1]}$. Hence oritatami system can yield only a finite structure whose size is $O(n^2)$ in $\delta = 1, \alpha = 4$.

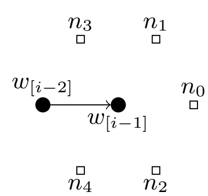


Fig. 22. $\alpha = 4$: when $w[i]$ is stabilized

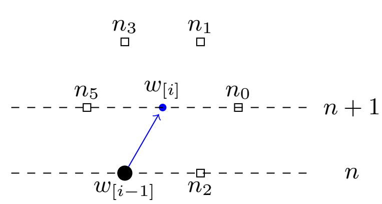


Fig. 23. the first bead out of $\hexagon^{n}_{w[-n+1]}$

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