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, when 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 $\texttt{A} \to \texttt{U}$, $\texttt{G} \to \texttt{C}$, $\texttt{C} \to \texttt{G}$, and $\texttt{T} \to \texttt{A}$ 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;

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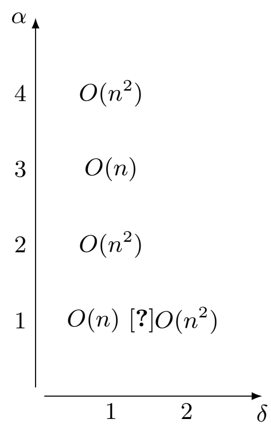


Fig. 1. Summary of the results.

- bounds on the size of the primary structure or of the attraction rule set;
- 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 $b_1, \ldots, b_n \in \Sigma$. The *length* of w is denoted by $|w|$, that is, $|w| = n$. For two indices i, j with $1 \le i \le j \le n$, 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 $k \ge 1$, $w[1..k]$ 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 N_p^d denote the set of points which lie in the regular hexagon of radius d centered at the point p. A directed path $P = p_1 p_2 \cdots p_n$ in $\mathbb{T}$ is a sequence of *pairwise-distinct* points $p_1, p_2, \ldots, p_n \in V$ such that $\{p_i, p_{i+1}\} \in E$ for all $1 \le i < n$. 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 $H \subseteq \big\{\{i, j\} \bigm| 1 \le i, i+2 \le j, \{P[i], P[j]\} \in E\big\}$. 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. 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 the second half of this paper, we consider 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 $\text{degree}(i) = |\{j | (i, j) \in H\}| > \alpha$ 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* $\mathrm{DTIME}(n^3)$.

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 $\mathrm{P} \subsetneq \mathrm{EXP}$, 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, an oritatami system can fold upon the seed of size n only the first $9n$ beads of a transcript deterministically. 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 $\alpha = 1$, 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. 14).

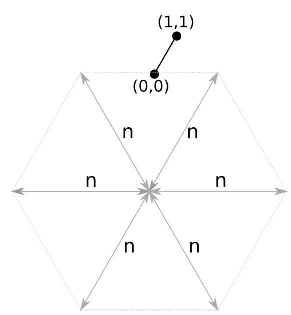
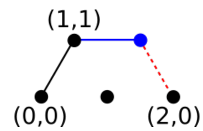


Fig. 2. N_p^n and the position $(1, 1)$ of the first bead fixed outside of it.

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 inert, 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 $i+2+m \to (2+m, 2)$, $i+3+m \to (2+m, 1)$.

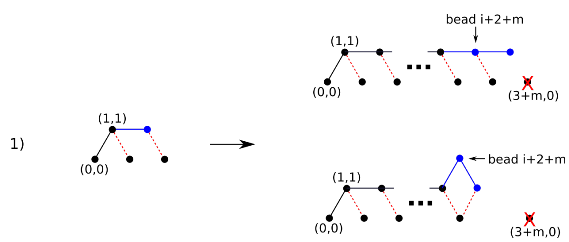


Fig. 3.

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.

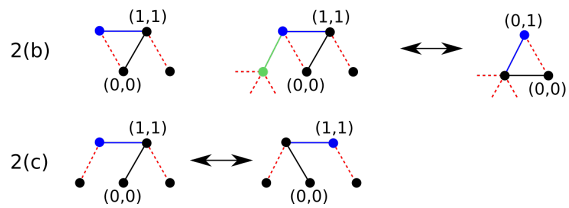


Fig. 4.

4.2 In the case of $\delta = 3$

We discuss when the length of seed is n. If the length of seed is n, the seed will be in an equilateral hexagon with a radius of n when it is given. We will begin our disscussion by considering the moment when a first bead is fixed on a side of an equilateral hexagon with a radius of $n+1$. Let us assume that a fixed bead on a side of an equilateral hexagon with a radius of n is able to make a hydrogen bond. If it is able to make only two hydrogen bonds, it will be nondeterministic because there are two possibilities that it makes two structures in Fig.5. Therefore, it needs to make three hydrogen bonds to determine the only structure.

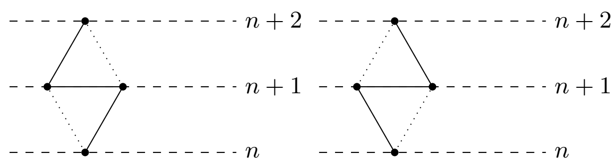


Fig. 5.

There are the two cases in which a first bead is fixed on a side of an equilateral hexagon with a radius of $n+1$ and it makes three hydrogen bonds in Fig.6. If it makes three hydrogen bonds once such as Fig6., it will make three hyrogen bonds forever to be deterministic. This becomes nondeterministic finally, such as in Fig.7., when it reaches a corner of an equilateral hexagon. Thus, the fixed bead on a side of an equilateral hexagon with a radius of n has to make a hydrogen bond with a bead in an equilateral hexagon.

Then, we will discuss the moment after the first the is fixed on a side of an equilateral hexagon with a radius of $n+1$. Let us assume that the bead is able to make a hydrogen bond. If it is able to make only two hydrogen bonds, it will be nondeterministic because there are possibilities that it makes two structures in Fig.8. Hence, it needs to make three hydrogen bonds to determine the only structure. It needs to be a right or left figure in Fig.9. to make three hydrogen

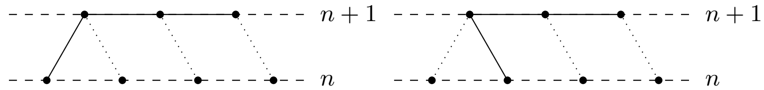


Fig. 6.

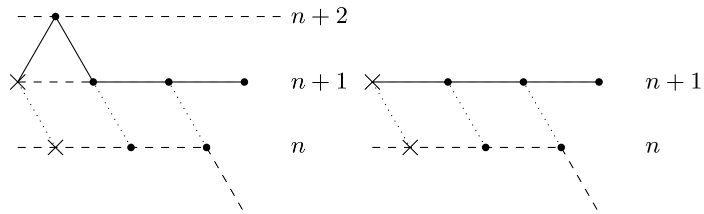


Fig. 7.

bonds.

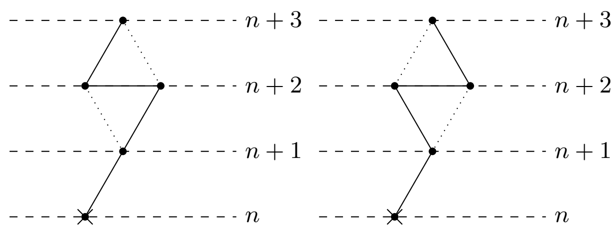


Fig. 8.

If it makes three hydrogen bonds once such as Fig.9., it will make three hyrogen bonds forever to be deterministic. This becomes nondeterministic finally, such as in Fig.7., when it reaches a corner of an equilateral hexagon. Therefore, the first fixed bead on a side of an equilateral hexagon with a radius of $n+1$ has to make a hydrogen bond with a molecule on a side of an equilateral hexagon with a radius of n.

Accordingly, it is Fig.10. when a first bead is fixed on a side of an equilateral hexagon with a radius of $n+1$.

It has to be a right or left figure in Fig.6. when the first bead fixed on a side of an equilateral hexagon with a radius of $n+1$ make a hydrogen bond with a bead on a side of an equilateral hexagon with a radius of n. Fig.6. becomes nondeterministic finally, such as in Fig.7., when it reaches a corner of an equi-

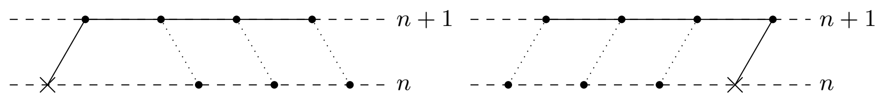


Fig. 9.

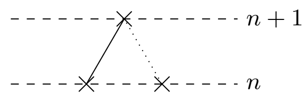


Fig. 10.

lateral hexagon. It is clear that all beads on a side of an equilateral hexagon with a radius of $n+1$ has to make a hydrogen bond with a bead on a side of an equilateral hexagon with a radius of n. It is impossible to fix molecules on a side of an equilateral hexagon with a radius of $n+2$ and determine the only structure when there are only beads which are able to make a hydrogen bond in an equilateral hexagon with a radius of n.

5 Case of delay 1

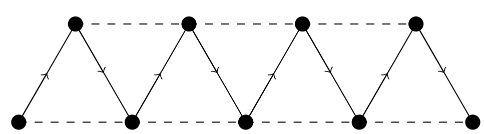


Fig. 11. zig-zag conformation

5.1 Introduction

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

Let Ξ be a deterministic oritatami system of delay 1 and arity 2. Assume its seed σ consists of n beads. For $i \geq 0$ let C_i be the unique elongation of σ by $w[1..i]$, that is, foldable by Ξ. Hence $C_0 = \sigma$.

Let us consider the stabilization of the i-th bead a_i upon C_{i-1}. The bead cannot collaborate with any succeeding bead $w[i+1], w[i+2], \cdots$ at delay 1. There are just two ways to get stabilized at delay 1. One way is to be bound to another bead. The other way is through a *tunnel section*. A tunnel section consists of four beads that occupy four neighbors of a point (Fig.3). Accordingly, how they are stabilized can be described by a binary sequence S of b's (bound) and t's (tunnel section); priority is given to t, that is, $S[i] = t$ if the i-th bead w_i is stabilized not only by being bound but also through a tunnel section.

Assume that four of the six neighbors of a point p are occupied by beads $a_{j_1}, a_{j_2}, a_{j_3}, a_{j_4}$ while the other two are free. We call such a point p the *inside of a tunnel* and points p' the *entrance of a tunnel* except when p' is inside of a tunnel. If the beads $w[i-2]$ and $w[i-1]$ are stabilized respectively at one of the two free neighbors and at p one after another, then the next bead $w[i]$ cannot help but be stabilized at the other free neighbor. In this way, $w[i]$ can get stabilized without being bound.

We say that point p is reachable from a conformation C if there exists a directed path P' from the last point of C that does not cross the path of C. We define *binding capability* with reachable.

Definition 1 (binding capability). *Let B_i be $(\{(h,i)|^{\forall}h < i\} \cup \{(i,j)|^{\forall}j > i\}) \cap H$. Moreover, let R_i be a set of neighbors of $w[i]$ that are free and reachable from C_j where C_j is a conformation which stabilized until $w[j]$. The number of binding capabilities of a conformation C_j is denoted $\#bc(C_j)$ and is defined by $\sum_{k=-n+1}^{j} \min\{|B_k|, |R_k|\}$.*

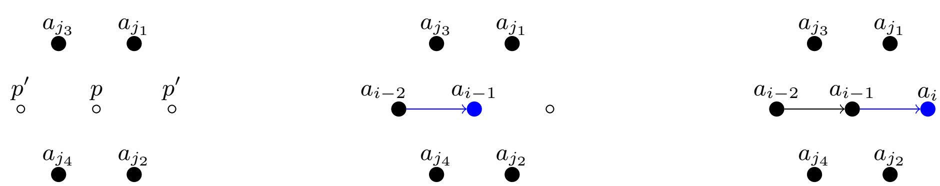


Fig. 12. Through a tunnel section

Theorem 2 (Tunnel Troll Theorem). *Let Ξ be a unary oritatami system of $\delta = 1, \alpha = 2$. If there are indices i and j such that $S[i..j+1] = bbt^{(j-i-1)}b$, then $\#bc(C_{i-1}) > \#bc(C_j)$ and if $S[i..j+1] = bt^lbt^mb \quad (l + m = j - i - 1)$, then $\#bc(C_{i-1}) > \#bc(C_j)$. On the other hand, at $\delta = 1$ and $\alpha \geq 3$, if $S[k] = t$, then $\#bc(C_{k-1}) > \#bc(C_k)$.*

Proof. Assume Ξ is deterministic. Each bead in the transcript is bound either inside a tunnel or outside. If a bead is stabilized inside a tunnel, then the position of successor is already decided either inside of a tunnel or outside. 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(A), obtuse(B) and acute(C) turn (Fig. 4), and we will consider each of those.

Lemma 1. *For unary transcripts at $\delta = 1$, if a bead has no free hand, then at least $\alpha + 2$ of its neighbors have to be occpied.*

Lemma 2. *Let Ξ be an oritatami system at $\delta = 1, \alpha = 2$. Assume Ξ stabilizes the transcript until $w[i-1]$. If $w[i]$ is stabilized at an entrance point of tunnel A or B, then $\#bc(C_{i-1}) > \#bc(C_i)$.*

Lemma 3. *Let $w[i]$ be a bead which is stabilized at the exit of a tunnel. At $\delta = 1, \alpha = 2$, if we assume $S[h..i+1] = bt^{(i-h)}b \quad (h < i)$, then $\#bc(C_{h-1}) \geq \#bc(C_i)$ and $\#bc(C_{i-2}) \geq \#bc(C_i)$. On the other hand, if we assume $S[k] = t (k \leq i)$ at $\delta = 1, \alpha \geq 3$, then $\#bc(C_{k-1}) > \#bc(C_k)$.*

Lemma 4. *Let Ξ be a unary oritatami system of $\delta = 1, \alpha = 2$. We assume $S[h..i+1] = bt^{(i-h)}b \quad (1 < h < i)$. If at least one of $w[h+1..i]$ is stabilized by tunnel C, then $\#bc(C_{h-3}) > \#bc(C_{h+1})$ and $\#bc(C_{h-3}) > \#bc(C_i)$.*

Let us first consider cases of $\delta \geq 3, \alpha = 1$. These cases are clearly true because of lemma3.

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 lemma2, if $w[h+1]$ is stabilized by tunnel A or B, then $\#bc(C_{h-1}) > \#bc(C_h)$. Also, According to lemma4, 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 lemma3. 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 $\#bc(C_{i-1}) > \#bc(C_j)$. □

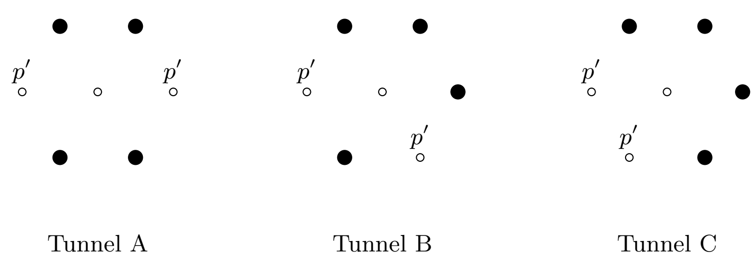


Fig. 13. All possible tunnel sections: straight, obtuse turn, and acute turn

Proof (lemma 1). Any transcript bead has predecessor and successor except for the first and last beads. If the bead does not have any free hand, then it uses hands with α neighbors. Thus, lemma 1 is clearly true.

Proof (lemma 2). Fig.5 exhibits all the three kinds of entrance of tunnel A, B. Let $w[i]$ be stabilized at an entrance point of Tunnel A or B. All cases are $\#bc(C_{i-1}) > \#bc(C_i)$ as follows.

- Case of t_0
  Let us consider points n_3, n_4. At least one of the points n_3 or n_4 is free because if both of them are occupied, p' is inside of tunnel. If n_3 is free, then p' has to be bound to a bead other than n_1 to deterministically stabilize. In this situation, at least three neighbors of n_1 are free, that is, n_1 has at least one free hand from lemma 1. Hence, p' must be bound to n_1. Thus, a case of t_0 consumes two hands and it does not supply any binding capabilities.
- Case of $t_{\pm 60}$
  In this case, too, n_4 or n_5 is free. If n_5 is free, p' has to be bound to n_1 or n_2. If n_5 is occupied, then n_4 is free. This time, by n_2 has some free hands so p' has to be bound to n_2.
  In this situation, p' is able to supply a binding capabilities which could bind a bead into n_4 or n_5. However, n_2 and n_3 are part of a contiguous conformation. According to Jordan curve theorem, any successors of p' cannot reach a point n_4 or n_5 so this capability is inactive. Thus, in the case of $t_{\pm 60}$ $\#bc(C_{i-1}) >$ $\#bc(C_i)$.
- Case of $t_{\pm 120}$
  Binding capabilities that p' supplies are inactive according to Jordan curve theorem on n_1 and n_2. Moreover, p' has to be bound to one of n_3, n_4, n_5 in order to deterministically stabilize. Thus, in the case of $t_{\pm 120}$ is $\#bc(C_{i-1}) >$ $\#bc(C_i)$.

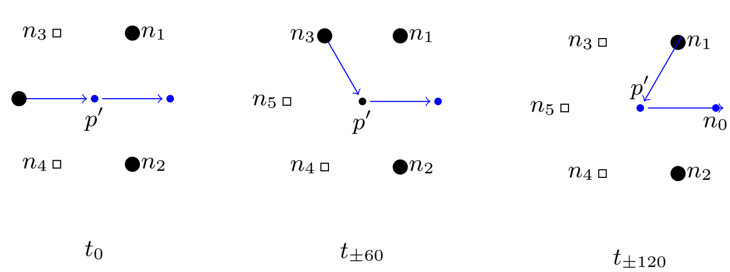


Fig. 14. Direction into a entrance

Proof (lemma 3). Fig.6 exhibits all the two kinds of exit of tunnel. At least one of points n_1 or n_2 is free because if both of them are occupied, p' is inside of tunnel.

$\delta = 1, \alpha = 2$
Let Ξ be a unary oritatami system at $\delta = 1, \alpha = 2$. We assume $S[h..i+1] =$

$bt^{(i-h)}b \quad (h < i)$ and let a be $\#bc(C_{i-2}) - \#bc(C_{i-1}) = a$. Then, $\#bc(C_i) - \#bc(C_{i-1}) \leq a$ as follows. Also, if $i - h > 1$ and j is such that $h < j < i$, then $\#bc(C_{j-1}) \geq \#bc(C_j)$ because all neighbors of $w[j]$ are occupied by beads forming the tunnel so that any $w[i+1..]$ cannot reach neighbors of $w[j]$. Thus, $\#bc(C_{h-1}) \geq \#bc(C_i)$ and $\#bc(C_{i-2}) \geq \#bc(C_i)$.

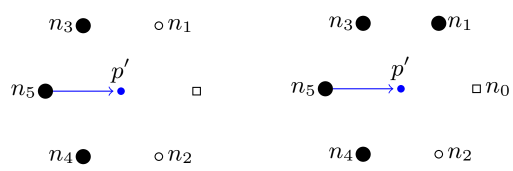
- Case of both n_1 and n_2 being free
  This case can be regarded the same as entrance. See Fig.6 (Left). Predecessor n_5 has to be bound to n_4 and n_5 because both of n_3 and n_4 have binding capabilities. Hence, $a \geq 2$. This time, $\alpha = 2$, that is, this case $\#bc(C_i) - \#bc(C_{i-1}) \leq a$.
- Case of n_1 is occupied
  See Fig.6 (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 $\#bc(C_i) - \#bc(C_{i-1}) \leq a$.

$\delta = 1, \alpha \geq 3$
Let Ξ be a unary oritatami system at $\delta = 1, \alpha \geq 3$. We assume $w[i]$ is stabilized at exit of tunnel. In all cases $\#bc(C_{i-1}) > \#bc(C_i)$. Moreover, if $S[k] = t(k \leq i)$, then $\#bc(C_{k-1}) > \#bc(C_k)$ because both sides of the path p in Fig.7 (n_1, n_2) have two free points and one of n_1, n_2 is not the predecessor so that it has hand and moreover that $w[k]$ supplies any binding capabilities because its neighbors are occupied by beads of tunnel.

- Case of n_1 and n_2 are free
  In $\alpha \geq 3$, if three neighbors of a bead leave, then it can supply two binding capabilities. Therefore predecessor n_5 has to be bound n_3 and n_4, and p', too. In this case, at least four bindings are consumed and at most two are added. Thus, it consumes some binding capabilities, overall.
- Case of n_1 is occupied
  In this case, n_4 leave at least two bindings and n_3, n_1 also leave at least one binding. Therefore n_5 has to be bound n_3 and n_4, and p' also has to be bound n_1 and n_4. In this case, at least four bindings are consumed and at most two are added. Thus, it consumes some binding capabilities, totally.

Proof (lemma 4). 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 lemma3 $\#bc(C_{h+1}) \geq \#bc(C_i)$. Thus, $\#bc(C_{h-3}) > \#bc(C_{h+1})$ and $\#bc(C_{h-3}) > \#bc(C_i)$.



Point n_1 and n_2 are free   Point n_1 is occupied

Fig. 15. Exit of Tunnel

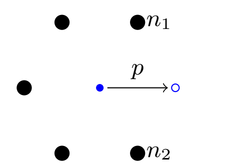


Fig. 16. Inside tunnel

Case of $S[h-1..h+1] = tbt$ Fig.8 exhibits all the two kinds of stabilization depending on structures of tunnel C.

- Left of Fig.8
  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.8
  These cases are divided on number of capabilities that $w[h-1]$ consumes.
  - $w[h-1]$ does not consume any bindings
    According to lemma3, $\#bc(C_{h-3}) \geq \#bc(C_{h-1})$ 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 $\#bc(C_{h-1}) > \#bc(C_{h+1})$.

Case of $S[h-1..h+1] = bbt$ Let us consider number of consumed bindings by $w[h-1]$ (Fig.9).

- $w[h-1]$ consumes one binding
  In this situation, $w[h-1]$ supplies one active binding whereas $w[h+1]$ consumes this binding. In addition, $w[h]$ has to bound to one of n_1, n_2, n_3. Thus, in this cases consume some binding capabilities.

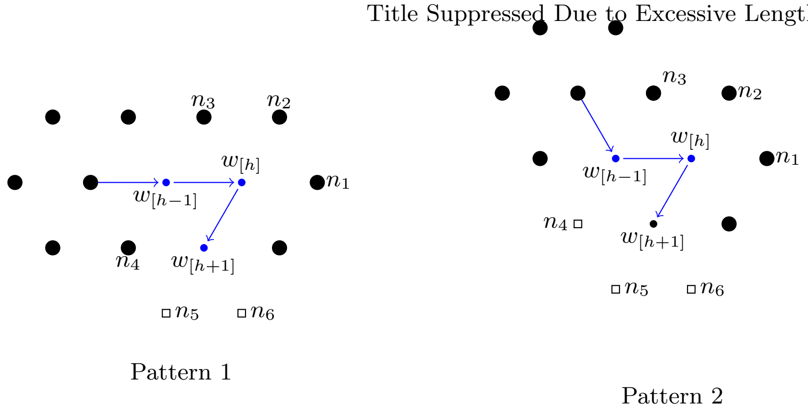


Fig. 17. Case of $S[h-1..h+1] = tbt$

- $w[h-1]$ consumes two bindings
  In this case, $w[h-1]$ already consumes two binding. $w[h]$ has to be bound. $w[h+1]$ supplies at most two bindings. Thus, in this cases consume some binding capabilities.

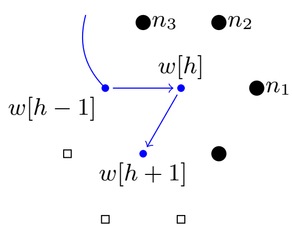


Fig. 18. Case of $S[h-1..h+1] = bbt$

5.2 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.10. $w[i-1]$ 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.

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

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

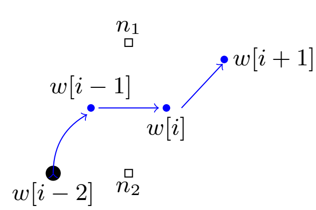


Fig. 19. Case of $S[i]$

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 $\mathcal{O}(n)$.*

Lemma 5. *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 1 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.11 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 lemma5. n_3 and the point which is stabilized $w[i]$ are free so that n_1 has some bond by lemma1. 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 lemma1, 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 lemma5, n_2 has to be occupied because n_4 is free. Also n_0 has to be occupied from lemma1. 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 lemma1. 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 lemma5, n_0 has to be occupied. n_1 has to be also occupied because of lemma1. 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.

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 $\mathcal{O}(n^2)$.*

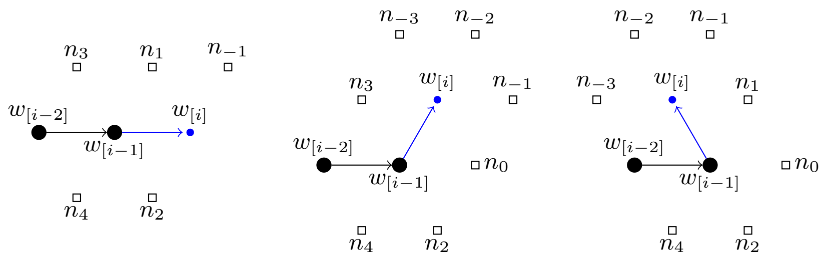


Fig. 20. All possible directions of $w[i]$: straight, obtuse, acute.

Lemma 6. *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.12. According to lemma1, 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 lemma6, 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.13. 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 $\mathcal{O}(n^2)$ in $\delta = 1, \alpha = 4$.

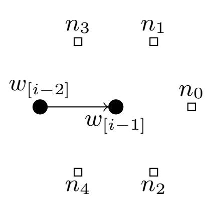


Fig. 21. $\alpha = 4$: when $w[i]$ is stabilized

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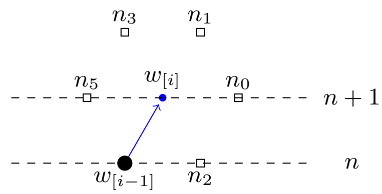

Fig. 22. the first bead out of $\bigcirc^{n}_{w[-n+1]}$

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